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access
NCSA newsletter
December 1987, Vol. 1 No. 5

Industrial Partners Program

NCSA Operations Staff. Top Photo: Remote Access Operations left to right—Joel Replogle, Susan Vinson, Mike Smith, Steve Crumb, Charlie Catlett. Left Photo: IRC Operations left to right—(back row) Dan Brady, Sue Lewis, Patsy Barnett, Ginger Winckler, Randy Butler, (seated) Gerry Quinn, Mike Aper. Right Photo: Supercomputer Operations left to right—Rich Brown, Walter Kreiling (on floor), Robert Wilson, Metaxia Lianos, Greg Schumacher (standing), Doug McCarthy , Mary Lou Young, Amy Swanson. See the article on page 7. (Photos produced by NCSA Electronic Media Services.)

ELI LILLY AND COMPANY BECOMES NCSA'S THIRD INDUSTRIAL PARTNER

Eli Lilly and Company has joined NCSA's Industrial Partners Program, NCSA Director Larry Smarr announced November 12. The Indianapolis-based pharmaceutical company signed a four-year $3.5 million agreement in which Lilly researchers and computer managers will receive training at NCSA and work closely with NCSA scientists and consultants.

"The application of supercomputing to drug design is a field that is just beginning to open up," Smarr said. "This agreement will bring one of America's premier pharmaceutical companies into a day-to-day working relationship with one of the most advanced scientific computing facilities in the world." That interaction, he said, should speed up development in the pharmaceuticals field.

Mel Perelman, president of Lilly Research Laboratories, said the agreement reflects Lilly's commitment to build "scientific resources and technological capabilities in order to continue to develop innovative products." Lilly is a research-based organization that develops, manufactures, and markets pharmaceuticals, medical instruments, diagnostic products, and agricultural products.

The agreement, which begins January 1, will locate Lilly researchers at NCSA to work on company projects. NCSA staff will provide training and research assistance and establish high-speed data links to off-campus Lilly facilities. Also outlined in the agreement, NCSA will add a computational chemist and computational biomolecular scientist to its staff to be available to Lilly for consultation.

Lilly is NCSA's third industrial partner. Eastman Kodak, Inc. joined the NCSA Industrial Partners Program in August 1986, and Amoco Corporation became the center's second industrial partner several months ago.

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Center Activities

FORTRAN 8X PUBLIC COMMENT PERIOD

A draft of the proposed revision of the ANSI Fortran Standard has been released for public comment during the period October 23, 1987 to February 23, 1988. There has been some controversy surrounding this revision, with proponents and opponents in both the user and vendor communities. The number and nature of comments received could have a significant effect on the standard finally produced. That standard, in turn, should have a major impact on scientific computing in the 1990s. All Fortran users having opinions on this subject are strongly encouraged to submit official comments during the comment period.

The draft revision itself can be obtained at a cost of $50 from Global Engineering Documents (1-800-248-0084 East Coast and 1-800-854-7179 West Coast). The document is a large one, so it is recommended that you order early in order to give yourself as much time as possible to digest the material and comment on the document. Written comments should be sent to:

Public Comments for Dpans Fortran Revision
X3 Secretariat
Attn: Gwendy Phillips
Computer and Business Equipment Manufacturers Association
Suite 300
311 First Street, N.W.
Washington, DC 20001-2178

and to:

Public Comments for Dpans Fortran Revision
Board of Standards Review
American National Standards Institute
1430 Broadway
New York, NY 10018

Your comments will be formally acknowledged and you will eventually receive a formal written response from X3J3, the committee that developed the draft.

NCSA users seeking clarification or other information about the draft prior to submitting their comments may wish to contact Kurt Hirchert, NCSA consultant, at the address: **hirchert@newton.ncsa.uiuc.edu**. Kurt has been a member of X3J3 since 1979 and should be able to answer any questions you may have about the draft.

— Kurt Hirchert

NCSA TRAINING PROGRAM REVISED

In an effort to bring more intensive, high quality training on the NCSA supercomputers to more of our remote users, the NCSA user's training program is being revised. The new program will begin in January 1988. Questions about the new program may be directed to: Alan Craig, NCSA training coordinator, at: `training@ncsavmsa`. As always, you can keep abreast of training news by typing `help training` on either the CRAY or the front-end VAX.

NCSA USAGE REPORT

NCSA has experienced steady growth in allocations and usage since opening to the national community on January 15, 1986. Beginning with a small number of "shakedown" friendly users, there are now more than 600 projects allocated with over 1500 user signons. Although the capacity of the CRAY computer more than doubled in November 1986 with the replacement of the original X-MP/24 computer with the current 8.5 nanosecond clock X-MP/48, the machine is now fully utilized with occasional periods of noticeably degraded responsiveness and throughput for individual users. The number of tasks competing for the CPU and memory frequently exceeds 80. This article details NCSA's growth in usage and attempts to identify some characteristics of that usage with the intent to inform and educate NCSA users how best to get their work done in this environment.

Figure 1 shows the monthly total CPU time (CPU hours) delivered to users and staff. The large jump in November 1986 was caused by the introduction of the CRAY X-MP/48 computer. Although the total allocation of the machine was less than the time available, there was a small number of users able to use time at a higher rate than their allocation rate, which kept the machine nearly fully utilized. Figure 2 shows a steady increase with as yet no apparent slowdown in the number of users obtaining various amounts of the available CPU time. The number of users obtaining more than 100 CPU hours per month has held to a fairly constant number of 2 to 5 throughout the life of the center, while the numbers of users in the 10-100 CPU hour group, the 1-10 hour group, and the 1 minute-1 hour group have all risen steadily. This growth indicates that new users are able to get accounts on the NCSA system and obtain access to significant CPU resources.

Figure 3 shows the amount of CPU time (CPU hours) delivered to users. In general over half the CPU time delivered is to users who use between 10 and 100 CPU hours.

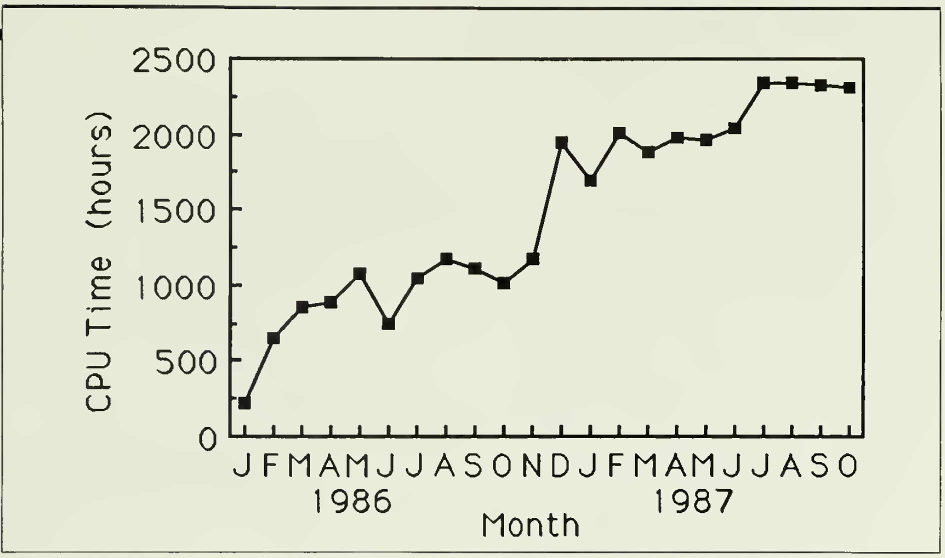


Figure 1. Total CPU Time Delivered to NCSA Users and Staff Each Month, January 1986-October 1987.

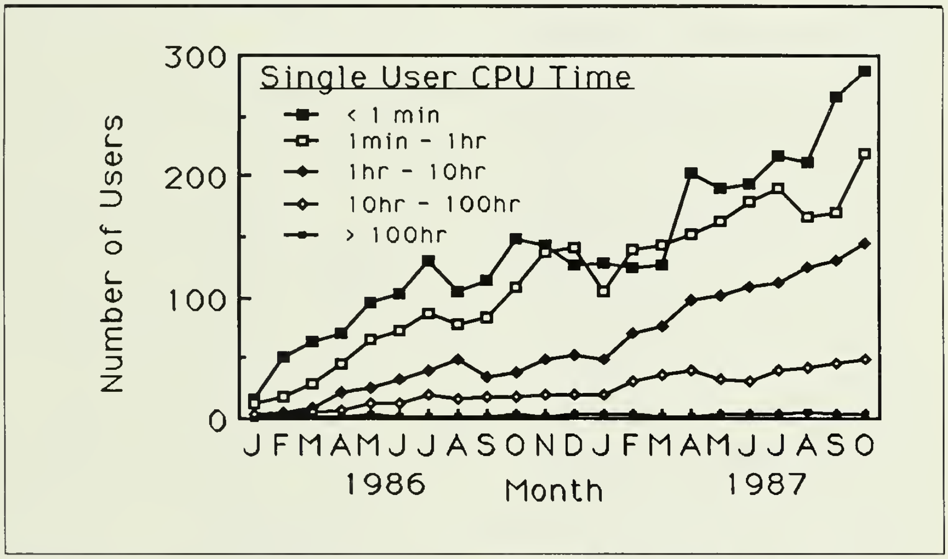


Figure 2. Number of Users in Specified Categories for Each Month, January 1986-October 1987.

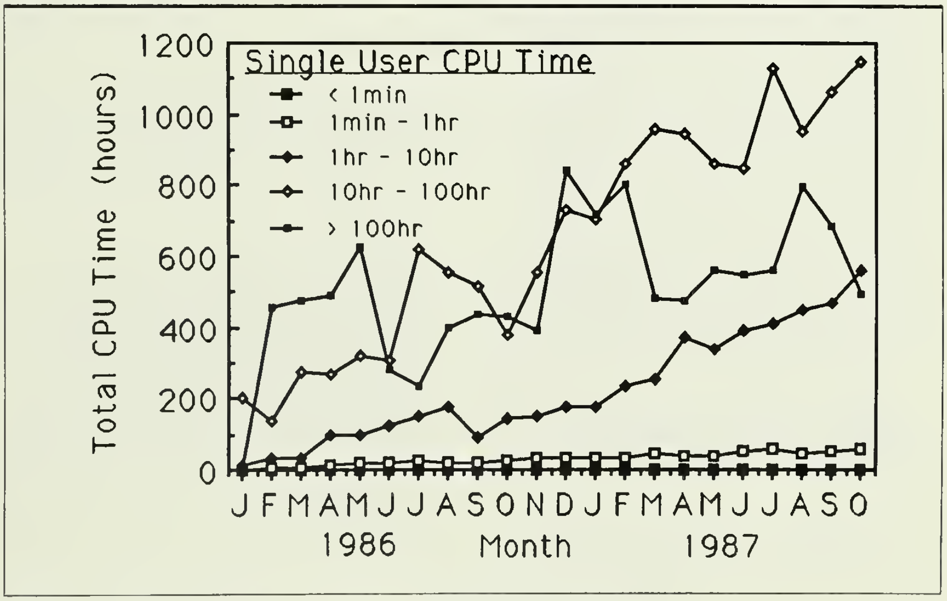


Figure 3. CPU Time Delivered to Users in Specified Categories.

Establishing Priorities

What is the implication of a fully utilized machine in which there is an increasing number of users? How is a system administrator to determine when a machine is over-allocated or "saturated"? One method is to look at the average priority of the jobs running on the system. A significant difference between CTSS and many mainframe batch operating systems is that CTSS gives the user total control over job priority, independent of the resource requirements of the job. It is this feature, combined with a fully utilized machine, that brought on June 1, 1987 an introduction of a charge against allocation based on the user-selected priority for all jobs run. Since that date, the average priority of charged CPU time has risen fairly steadily to its current level of approximately 0.9. It is interesting to look at the distribution of job priorities both over time and as accumulated over the month to learn how users bid for priority and get some feeling for the demand on the CRAY computer.

Figure 4 shows the distribution of CPU time used during the month of October 1987 versus job priority. What is immediately obvious from this distribution is that instead of any sort of normal distribution driven by user demand, there is a pronounced peak at priority 1.0, the default CTSS command priority. This suggests that user convenience in accepting the default priority, rather than cycle demand or machine load level, is driving the choice of job priority. This large peak demand for priorities above the 0.9 average reduces the correlation between priority selected and cycles delivered, causing a charge rate to the user's account of 10-20 percent more than necessary for getting virtually the same service, and reducing the system response to users who want good response for short CPU bursts of interactive work. These people should ask for a high priority.

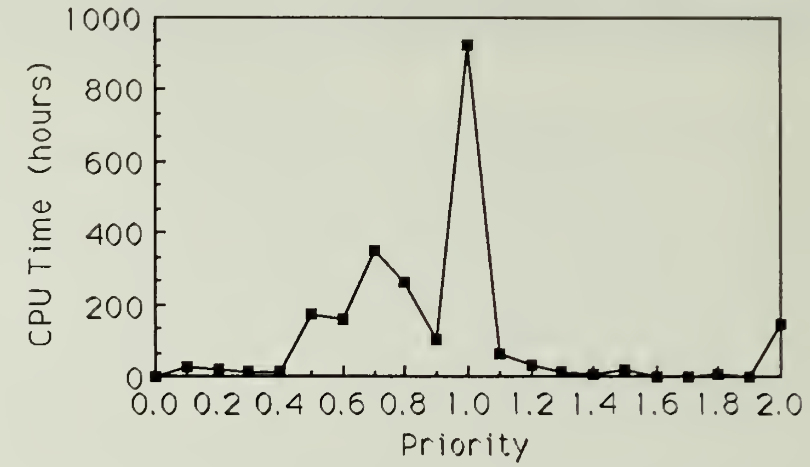


Figure 4. CPU Time Used Versus Priority During October 1987.

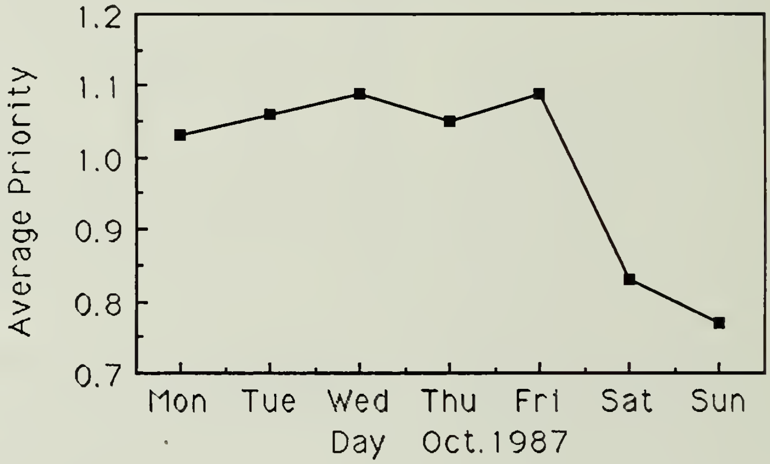


Figure 5. Average Daily Priority During October 1987.

Setting Time Limits and Priorities

In addition, often a user asks for a high priority to run through an interactive initialization segment of the job, then logs off, leaving the job running unattended without first reducing the priority. Remember that the priority of a job can be specified on the CTSS command line by including the time limit and priority following a slash after the program name and any arguments as follows:

ctss_command / time priority

where ***time*** is in minutes and ***priority*** can range between 0.1 (low priority and service) and 2.0 (high priority and service). After a job is executing, its time limit may be changed by pressing **CTRL-E** and then entering:

```
tl nnn.nn
```

where *nnn.nn* is a new time limit in minutes. If the time is omitted, the system responds with the current time left (`tl`) for the job. Likewise, the job priority may be changed while the job is executing by pressing **CTRL-E** and then entering:

```
pc m.mm
```

where *m.mm* is the new priority. If a priority is omitted, the system responds with the current job priority. The best method of determining the most efficient priority is probably trial and error with your application. The mix of priorities of jobs currently executing can best be seen with the `dg` command. `dg` shows the 28 highest priority jobs executing and currently in memory. The `dg mem` command shows the 28 highest priorty executable jobs that are currently waiting to get into memory. In general, choose a middle to low priority from the observed range if you have a long running job and are not primarily concerned with fast turnaround (for example for an overnight or weekend job.) Use the `CTRL-E tl` or `dg` commands to monitor the CPU time obtained over a period of time, and adjust the priority as necessary. Another way of obtaining a given amount of service at a lower priority, and thus lowering the charge, is by running the job at the off hours of late night or weekend. Not only is the average priority lower at these times, but there tends to be fewer jobs competing for the CPUs.

Figure 5 shows the average priority for each day of the week in October 1987. Figure 6 shows the average priority as a function of time of day for week and weekend days during this same period. The average number of logged-in users is shown in Figure 7. Note the correlation between the number of users logged in and the average job priority of Figures 6 and 7. It seems clear that although all four CPUs of the CRAY computer are busy at all times, there are periods when better throughput or lower charge can be realized. NCSA is currently developing some tools, including a batch submission facility and system job scheduler modifications to ensure good response and throughput for those users who need it. Until these tools are available, all users can help by running at the lowest priority required to obtain the desired system service and running long jobs at night or on the weekend.

— **Lex Lane**

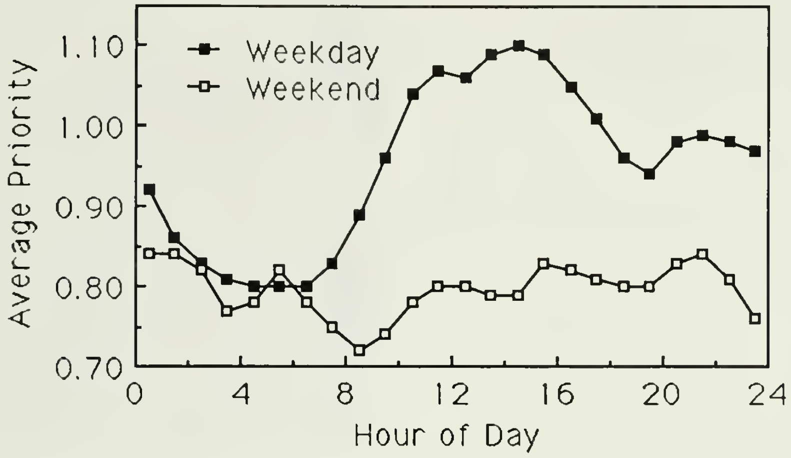


Figure 6. Average Priority Based on Time of Day During October 1987.

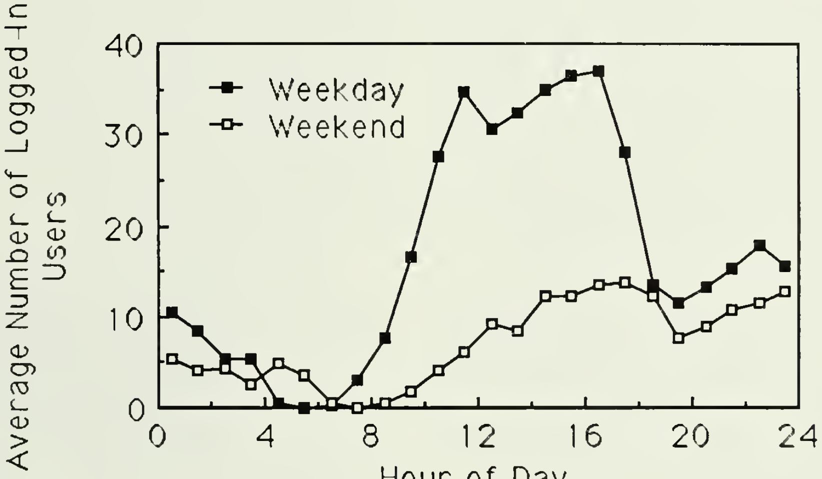


Figure 7. Average Number of Logged-in Users Throughout the Day During October 1987.

SECOND AFFILIATES TRAINING WEEK HELD

The affiliates were rounded up for their group photo.

The NCSA Academic Affiliates Program expanded into a number of new areas at the recent training session held at the Interdisciplinary Research Center. In addition to training on CTSS, vectorization, workstations, networking, graphics, and updates in all these areas, new sessions were included on the upcoming CRAY 2. Also discussed were new developments and opportunities in parallel processing and NCSA's second Alliant FX/8. The affiliates beta tested the newest version of the multi-session NCSA Telnet program for the Mac and IBM PC and heard about a number of other new software offerings for graphics and remote users.

Representatives from 25 affiliate institutions, 18 of which were new to the program, attended the training session October 5-9. The campuses represented ranged from Georgia to Alaska and from Delaware to California. Each new affiliate institution received a Mac SE from Apple Computer, Inc., which was used during the training session. Most people promptly loaded their Macs with public domain software before taking the machines back to their colleges.

While much of the time in class was spent on technical aspects of the NCSA system, a good deal of the remaining time was devoted to discussions between staff and affiliates analyzing the NCSA Academic Affiliates Program and the spectrum of services NCSA provides. This was one of the most interesting and rewarding sessions for NCSA staff members and affiliates, giving both sides an idea of how the program has developed over the last few months, and a chance to suggest improvements for the future.

Mike Norman, NCSA research scientist, gave the group an overview of new developments in visualization tools and networking that will eventually allow remote researchers to work more effectively. Speaking at a dinner held for the affiliates on Monday, October 5, Norman described his Sun/3-based Imagetool for color raster image display, animation, and analysis. Dinners, organized and otherwise, took up many of the participants' evenings and provided a number of opportunities for NCSA staff members and affiliates to get to know each other and exchange ideas.

NCSA staff talks, demonstrations, and discussions ranged from network troubleshooting to using the new HyperCard on the Mac to animate images pulled directly off the CRAY computer. Many of the affiliates commented that seeing what was new and being shown how to use it constituted one of the most rewarding aspects of the week.

Ahmed Sameh talks to the academic affiliates about parallel processing and the CSRD CEDAR project.

Bob Wilhelmson, NCSA associate director, gave a well-received talk and demonstration on the uses of simulation and scientific visualization techniques in the study of thunderstorms.

The affiliates also heard from speakers on a variety of other interesting topics. These speakers included Dr. Ahmed Sameh, associate director for the Center for Supercomputing Research and Development (CSRD) at the University of Illinois. Sameh spoke to the attendees about the next generation of supercomputers, including a description of the CSRD CEDAR parallel processing project.

NCSA considered the week very successful and, according to the evaluations, the affiliates did too. The next affiliates session (to be held February 15-19, 1988) is an advanced or Phase 2 session, open to people who have attended an earlier Phase 1 session. The next Phase 1 session for affiliates with no prior training will be March 7-11, 1988.

Anyone interested in the Academic Affiliates Program should contact Joseph Hardin at (217) 244-0072; at BITNET address: `hardin@ncsavmsa;` or at Internet address: `hardin@ncsaa.ncsa.uiuc.edu`.

— Joseph Hardin

NCSA Profile

OPERATIONS GROUP TAKES RESPONSIBILITY

Research scientists may be regarded as the core of a supercomputing research center, but without the broad mission accomplished daily by NCSA's Operations Group, the research scientists might not have a supercomputer that is up and running. Operations makes sure the CRAY computer and the Interdisciplinary Research Center (IRC) at the University of Illinois' NCSA are functioning well and that NCSA's resources are available for its user community.

"Reliability is what we're held accountable for," said Mike Smith, NCSA manager of operations, systems administration, and facilities. Operations is split into three groups to handle its three areas of responsibility: Supercomputer Operations, IRC Operations, and Remote Access Operations.

Perhaps the most critical of these groups is Supercomputer Operations. It is responsible for staffing and maintaining the CRAY computer at all times. Mary Lou Young, systems administrator for the CRAY computer, said the CRAY computer's day begins at 7 a.m. after it is brought back online from block time maintenance. Utilization analysts spend from 7 a.m. to 3 p.m. monitoring disk space availability, validating users, maintaining systems utilities, and working on programming projects. In the afternoon, the swing shift takes over and performs similar functions, as well as answering after-hours consulting calls on the weekdays. At 11 p.m. the night shift monitors the CRAY computer, and at 3:30 a.m. operators warn users that the computer will be down for preventative maintenance at 4 a.m. and returned to normal operations by 7 a.m. Young said all three shifts also make tape file backups weekly to ensure the integrity of all critical disk-resident files.

In monitoring the system for errors, Young explained, "Most of the potential problems are avoided due to the computer utilization analysts' rapid response to various warnings given on the monitoring devices in the operations area." With CRAY usage increasing, Young said watching disk space is very important because sufficient disk space is crucial for proper system operation.

The IRC Operations group has a similar mission. At 5 a.m. IRC Operations brings down the network connections within NCSA's IRC for block-time maintenance on such hardware as the Alliant FX/8 or the IRC network. Working during this time avoids disturbing the network during prime usage. Once the system is back online, the IRC Operations group spends most of the day performing systems administration functions such as user logon maintenance and error detection and correction. IRC Operations also works with vendors in the planning, acquisition, installation, and maintenance of all the IRC's equipment.

Ginger Winckler, IRC operations administrator, called the group the "service arm for NCSA workstations." She said that as the center grows in terms of people and the number of computer systems, the group's responsibility is to ensure that the networks can handle the increased loads.

Operations' newest direction, Remote Access Operations (RAO), is charged with developing and servicing high-speed access to the CRAY computer for remote users. Charlie Catlett, coordinator of the new group, said RAO is responsible for network connections to Indiana University, a T1 network to the University of Illinois Chicago campus (this will serve as a supercomputer hub to the Chicago area), and a T1 line to Kodak Research Park in Rochester, NY. (Kodak is an NCSA industrial partner.)

RAO is presently developing a network to Amoco, a new industrial partner in Naperville, IL. The group also supports NCSA's major network connections (NSFnet and ARPANET) and does consulting work for NCSA users, staff, and visitors.

NCSA's Operations group as a whole has taken giant strides in the last year, Smith said. Over the past six months, the CRAY computer has had "on the average" a 99 percent overall system reliability. Young said NCSA's CRAY computer has had only three cold dead starts in its history, and two were attributed to a "difficult startup period we experienced with the arrival of the CRAY X-MP/48 computer." To better meet its responsibilities, Operations has doubled the size of its staff.

The toughest part of Operations' job is "being a specialist at everything, anytime of the day or night," Smith said. Key staff are required to carry a beeper with them at all times in case of an emergency. But these have not been used much, because the frequency of problems has gone down, primarily because of the amount of planning that goes into the installation of systems at NCSA.

—Phil Hattwick

Networking

MIDnet: A REGIONAL NETWORK IS BORN

A new regional NSF network is now connected to the NSFnet backbone via the NCSA/UIUC NSFnet node. MIDnet, managed by Doug Gale of the University of Nebraska, connects 12 midwestern universities to the NSFnet (see MIDnet map on page 8). The network supports the TCP/IP protocols. The TCP/IP protocols, standard on the NSFnet, allow users on hosts with access to the network to use Telnet (remote interactive login), FTP (file transfer program), and to send electronic mail to other NSFnet/ARPANET hosts.

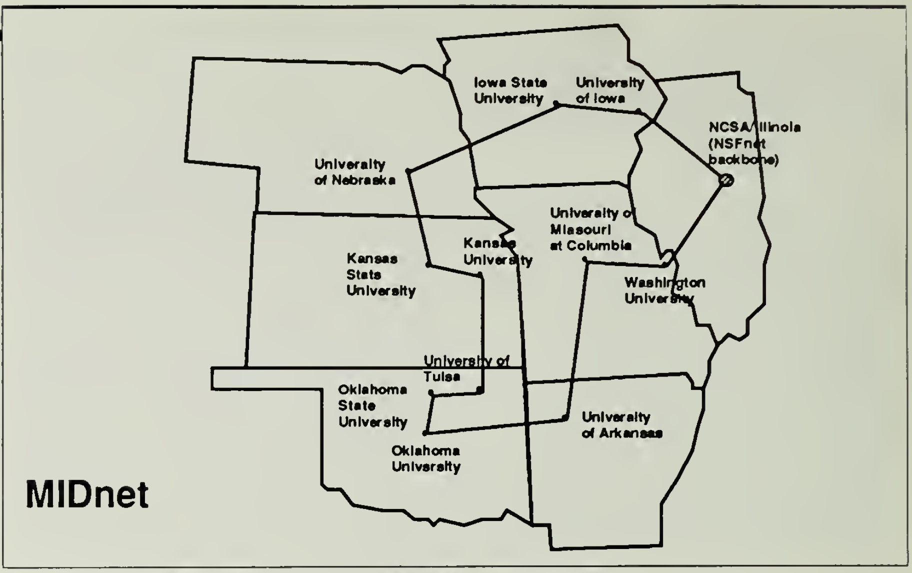
MIDnet is connected via 56Kbps circuits using Proteon P4200 packet routers. The circular topology provides two paths to the NSFnet from each MIDnet node. In general, a shorter path is used as a primary route, and a

Midnet continued on next page

Midnet continued from previous page

secondary path is used automatically in the event of a circuit failure on the primary path. This fault recovery is done automatically by the routers and is transparent to network users.

Users on MIDnet campuses should contact their local networking support personnel listed below for details on how to access MIDnet. (Electronic addresses were not available for all representatives.)



MIDnet connects 12 midwestern universities to the NSFnet.

School	Technical Representative	Institutional Representative
Iowa State University	Randy Dalhoff (515) 294-8693 `gr.rfd@isumvs.bitnet`	George Strawn (515) 294-3402 `gm.gos@isumvs.bitnet`
Kansas State University	Brick Verser (913) 532-6311 `bav@ksuvm.bitnet`	Mike Miller (913) 532-6311 `mhm@ksuvm.bitnet`
Oklahoma State University	Russ Teubner (405) 624-6301	Robert Gumm (405) 624-6301
	Paul Woods (405) 624-6301 `ppw@uccunx.uxx.okstate.edu`	
University of Arkansas	David Merrifield (501) 575-2901 `dm06900@uafsysb.bitnet`	Robert Zimmerman (501) 575-2901 `rz85099@uafsysa.bitnet`
	Dan Puckett (501) 575-2905 `dp06001@uafsysb.bitnet`	
University of Iowa	Larry Taylor (319) 335-5459 `bptlctpb@uiamvs.bitnet`	Lee Shope (319) 335-6042 `bptleepb@uiamvs.bitnet`
University of Kansas	Dave Nordlund (913) 864-4291 `nordlund@ukanvm.bitnet`	Jerome Niebaum (913) 864-4291 `niebaum@ukanvm.bitnet`
University of Missouri-Columbia	Ben Colley (314) 882-9730 `tpmaint@umcvmb.bitnet`	Otho Plummer (314) 882-8205 `ccplum@umcvmb.bitnet`
University of Nebraska-Lincoln	Mark Meyer (402) 472-5654 `marc@unlcdc3.bitnet`	Doug Gale (402) 472-5108 `doug@unlcdc3.bitnet`
	Dale Finkelson (402) 472-5032 `dmf@unl.csnet`	
University of Oklahoma	Jim White (405) 325-6988	Robert Shepard (405) 325-7234
	Richard Lewis (405) 325-6988	

— **Charlie Cattlet**

Software

NEW SOFTWARE MADE AVAILABLE

Following are summaries of articles that appear in this issue of ***data link***. These articles describe new NCSA software that is now available. If you do not receive ***data link***, but are interested in one of the following software articles, call NCSA at 217-244-0072 to get a copy of the article. If you want to receive ***data link*** on a regular basis, fill out the subscription form in this newsletter.

ELLPACK Mathematical Package

NCSA introduces a software package for solving elliptic boundary value problems for mathematical modeling projects. The package contains an extensive library of problem-solving modules and is a flexible tool for both experimenting with numerical methods and solving applications problems.

Improved Mass Utility for VMS

Changes have been made to the `nmass` article which appeared in the Vol. 1 No. 3 issue of ***data link***. This revised article contains a list of changes to the `mass` utility as well as a tutorial on using `nmass`.

New CFTLIB Installed

NCSA introduces the new version of CFTLIB, installed in early November. Differences in using the new version are identified.

PORT Math Library Made Available

You can now use the PORT mathematical subroutine library on the CRAY computer. PORT, developed by AT&T Bell Laboratories, incorporates the traditional areas of mathematical software, but does not include statistical routines. An overview of the features of the library is given.

SMPAK Makes Yale Sparse Matrix Package Available

This article describes how to call up the SMPAK collection of routines for solving linear equation systems with a large and sparse coefficient matrix. SMPAK uses Gaussian elimination without pivoting in its solution technique and uses a three-step solution process.

Using Gaussian 86 on the CRAY X-MP/48

Subroutines within Gaussian 86 which perform semi-empirical and ab initio molecular orbital calculations. A list of these routines and how to use them is given.

CHANGE TO MASS USAGE

NCSA users have asked for a simpler way to use CFS, so on December 14, 1987, NCSA began automatically issuing the `create` command for all new userids. This change means that a new user does not need to create a root directory before saving any files, as described in the NCSA *User's Guide*, Version 1.1.

— **Scott Lathrop**

CHANGE TO VAX SIGNONS

To simplify the use of the scratch disk on the VAX, NCSA is now automatically generating a scratch directory for every new userid that is created.

The scratch directory that is created is of the form:

```
disk$scratch:[scratch.userid]
```

where ***userid*** is your userid.

In addition, the logical `scratch` is being added to the `login.com` file for every new userid. This enables you to enter **scratch** and automatically have the working directory become your scratch directory. To return to your home directory, enter **home** or **set default sys$login**.

— **Scott Lathrop**

NCSA CRAY/SUN DISTRIBUTED EMACS

A full screen editor is now available on the CRAY X-MP, for users of Sun workstations with network access to the CRAY computer. It is a derivative of MicroEMACS, a fairly powerful and portable editor available in resident form on a wide variety of micro- and mini-computers. This distributed implementation allows editing in a network efficient manner on the CRAY computer.

Some features of the CRAY/Sun version include:

- Mouse support for cursor movement and cutting/pasting text. Use of the mouse minimizes the load on the network, sending far fewer packets than would be sent if only cursor keys were used.
- Function key support. Over 50 function keys are defined. A keyboard template is available, so you need not be familiar with Emacs command sequences. An additional 10 function keys may be defined by you.
- Direct use of TCP/IP for efficient and reliable operation.
- Pop-up operation of the editor window, leaving the login window for normal use of the CRAY computer.
- A login window which provides a VMS/ksh style command line editor and allows the definition of argumented macros. The command line editor uses Emacs keystrokes and function keys to be consistent with the full screen editor.
- Buffering of rapidly typed control keystrokes so that they are sent as a single packet.
- Multiple windows, files, and buffers.

The machines must be able to contact each other directly via Telnet. Currently, only the Sun version of the editor is available. However, if you are interested in attempting a port to another workstation, the source for the NCSA version is available. Interested parties should contact Roger Ove at **ove@newton.ncsa.uiuc.edu** or **14004@ncsavmsa** (BITNET).

MicroEMACS was originally written by Dave Conroy, and includes contributions from many people. Most notable among the contributors is Daniel Lawrence, who also maintains the source. This noncommercial implementation is derived from Lawrence's version 3.8, to which he holds the copyright.

For further information on NCSA CRAY/Sun Distributed Emacs, refer to this month's issue of ***data link***.

— **Roger Ove**

Visitors Program

New Mexico Astronomers at NCSA

Professor Jack Burns and research associate, Dr. Martin Sulkanen. (Photo produced by Steven Blakey, NCSA Electronic Media Services.)

The eternal quest for knowledge and understanding of the universe leads to infinite problems and possibilities. It is currently believed that within the centers of some galaxies there may be very large black holes, and that the black holes can produce thin collimated jets of gas that are beamed away from the galaxy. Professor Jack O. Burns and associate, Dr. Martin E. Sulkanen, astrophysicists in the Department of Physics and Astronomy at the University of Mexico, have been working on the properties of such jets during their participation in the NCSA Visitors Program.

Burns and Sulkanen, with the assistance of NCSA research scientist, Dr. Michael Norman, are using the CRAY computer to simulate these jets as they propagate in different background media to determine if the jets can be disrupted. Identifying the behavioral manifestations of these jets in different media can lead to greater understanding of the environment through which these jets travel. This may explain an observed species of jet that undergoes a sudden flaring and disruption as it propagates away from the galaxy.

There are three models to explain jet disruption that Burns and Sulkanen are currently investigating. One explanation is the jet collides with a massive cloud of interstellar gas, which deflects and "sprays" the jet. In the other two models the jet encounters a large and rapid increase in the pressure in the surrounding galactic gas. Such pressure changes may exist in gas that flows *toward* the galaxy's center by cooling, or in gas that flows *away* from the galaxy in the form of a "wind."[1,2]

As a first application of Mike Norman's hydrodynamic simulation code, ZEUS, to this problem, Burns and Sulkanen used the model in which the background wind undergoes a *shock,* a sudden change in its properties, as it reaches the galaxy's periphery. The issue in this case was to determine what would happen to the jet upon crossing the shock front. The results of these simulations indicated that the shocked wind is quite effective in flaring and disrupting the jets, although such a background is probably not appropriate for all of the observed jets. Burns and Sulkanen are now attempting to find similar jet disruption with the "cooling infall" model for the background gas.

Simulation of shock-disrupted galactic jet. (Photo produced by NCSA Scientific Visualization Program.)

A second project which Dr. Burns is working on is the observational counterpart to the jet disruption model. By taking data collected from the Very Large Array (VLA) radiotelescope located at Socorro, NM and analyzing the data with the NCSA CRAY computer, Burns is able to process the images into a very large map. Burns stated that "this is the only place in the world, currently, where one can process VLA images of this size." The experimental software that makes this possible, called WERONG, was developed by Dr. Bob Sault, from the Department of Astronomy at the University of Illinois.

Finally, one more project that Dr. Burns is working on is the mapping of large-scale structures in the universe. As Dr. Burns states in the July 1986 issue of *Scientific American,*[3] "clusters of galaxies make up enormous superclusters, which alternate in space with immense voids. Such structures were born in the high-energy interactions of the early universe."

Three potential models for examination of these phenomena have arisen. These are the isothermal, neutrino, and cold-particle models as described in Burns' article. Supercomputer simulations are being developed to ascertain "the distribution of rich clusters that might be expected in each model." Working in close association with Stefen Fangmeier of NCSA's Scientific Visualization Program and with the use of the Alliant FX/8, Burns is producing a

Astronomers continued on next page

Astronomers continued from previous page

three-dimensional visual comparison of the models with the observations.

Dr. Burns was the founder and first director of the Institute for Astrophysics at the University of New Mexico. The institute operates an observatory at Capilla Peak, NM. It is one of the highest in the U.S., employing a charged-coupled device camera attached to a 24-inch (0.6 meter) aperture telescope. In the proposal and planning stages is a collaborative arrangement to develop a multiple, large telescope observatory with the New Mexico Institute for Mining and Technology.

Professor Burns and Dr. Sulkanen will be returning to New Mexico sometime in December. They will be running ZEUS remotely from the University of New Mexico.

— **Pamela M. Salela**

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[1] Special thanks to Dr. Martin Sulkanen for writing this portion of the article, which describes the three models of jet disruption.

[2] For more detailed information on cosmic jets, see the article "Cosmic Jets," *Scientific American*, May 1982.

[3] Jack O. Burns, "Very Large Structures in the Universe," *Scientific American*, July 1986.

Visualization

APPLICATIONS FOR VISUALIZATION

NCSA has just completed its "friendly user " period for the visualization services and has established an application process so the national community may apply. Applications for this service will go through a review process similar to the process that is used to allocate time on the CRAY computer. NCSA has instituted a Visualization Review Board composed of nationally recognized visualization experts. The board will meet for the first time in late February to review the first set of submitted proposals. To be considered at the February meeting, applications must be received by January 25, 1988.

Scientists with supercomputer data that requires visualization through three-dimensional computer graphics and animation should send their name and address to **johnston@ncsavmsa** (BITNET address) or **johnston@newton.ncsa.uluc.edu** (ARPA Internet address) or on a postcard to:

Ronnie Johnston
133 Computing Applications Bldg.
605 E. Springfield Avenue
Champaign, IL 61820

Applications are in the process of being printed and should be available December 14. At that time, we will begin sending them out to those interested. Applications will be approved based upon the degree to which each project can contribute to new techniques in both visualization and the computational sciences.

VISUALIZATION PROGRAM WINS AWARD

The NCSA Scientific Visualization Program won the Special Award in Computer Graphics from AV Software International '87 and Nicograph Association of Japan for its entry of the "Project Sci-Vi" videotape. This award endows 500,000 yen to the winning program.

Originally made in July for showing at SIGGRAPH '87, "Project Sci-Vi" is a compilation of images edited from 13 NCSA visualization projects produced by the program from April 1987, (when the visualization program became operational) through July 1987.

Nancy St. John, manager of the Scientific Visualization Program, said, "This was our first submission to any competition. Hopefully, this award will be the first of many for our program as we bring to scientists computer graphics and animation software and hardware tools and techniques which until now were only available to the entertainment and commercial world."

VISITORS AT NCSA

Colleen Barton. Dec. 14, 1987-Jan 14, 1988 from Stanford University. Major area of interest: geophysics.

Ken Bishop. Sept. 27 - Dec. 15 from the University of Kansas. Major area of interest: petroleum engineering.

Jack Burns. July 1 - Dec. 30 from the University of New Mexico. Major area of interest: astrophysics.

Charles Evans. Nov. 12 - Nov. 23 from California Institute of Technology. Major area of interest: astrophysics.

John Hawley. Nov. 12 - Nov. 23 from University of Virginia. Major area of interest: astrophysics.

L. P. Hughston. Nov. 15 - Dec. 15 from Oxford University. Major area of interest: applied mathematics.

Mordecai Maclow. Nov. 30 - Dec. 12 from the University of Colorado. Major area of interest: astrophysics.

Martin Sulkanen. July 1 - Dec. 30 from the University of New Mexico. Major area of interest: astrophysics.

Eung Sun Lee. Nov. 16 - 17 from Georgia Institute of Technology. Major area of interest: computational mechanics.

Larry Tesler. Dec. 14, 1987-Jan. 14, 1988 from Apple Computer, Inc.

James R. Wilson. Nov. 2 - Nov. 7 from Lawrence Livermore National Laboratory. Major area of interest: astrophysics.

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Front-end VAX IP Address	ncsaa.ncsa.uiuc.edu (128.174.5.100) ncsab.ncsa.uiuc.edu (128.174.5.101)
NSFnet Problems (NSF Network Service Center)	617-873-3400 nnsc@nnsc.nsf.net
ARPANET Problems (SRI-Network Information Center)	800-235-3155 415-859-3695 nic@sri-nic.arpa

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data link Vol. 1 No. 5 Preview

CODE IMPROVEMENT USING CALMATH

This article describes how to apply CALMATH machine-language subroutines to speed up your CRAY programs.

ELLPACK MATHEMATICAL PACKAGE

NCSA introduces a software package for solving elliptic boundary value problems for mathematical modeling projects.

IMPROVED MASS UTILITY FOR VMS: NMASS

Changes to the `nmass` article in the Vol. 1 No. 3 issue of ***data link*** have been made.

NCSA CRAY/SUN DISTRIBUTED EMACS

NCSA introduces a CRAY full-screen editing program that runs on the Sun workstation.

NETWORK MAIL ON THE NCSA VAX

This article gives information on how to send mail to other networks using the gateway machines.

NEW CFTLIB INSTALLED

NCSA introduces the new version of CFTLIB installed early in November. Differences in using the new version are identified.

PORT MATH LIBRARY MADE AVAILABLE

You can now use the PORT mathematical subroutine library on the CRAY computer. PORT, developed by AT&T Bell Laboratories, incorporates the traditional areas of mathematical software, but does not include statistical routines.

SMPAK MAKES YALE SPARSE MATRIX PACKAGE AVAILABLE

This describes how to call up the SMPAK collection of routines for solving linear equation systems with a large and sparse coefficient matrix.

USING GAUSSIAN 86 ON THE CRAY X-MP/48

This article describes subroutines within Gaussian 86 which perform semi-empirical and ab initio molecular orbital calculations.

data link is a collection of technical articles for NCSA computer users. If you do not receive ***data link***, but are interested in one of the above articles, call NCSA at 217-244-0072 to get a copy of the article. If you want to receive ***data link*** on a regular basis, fill out the subscription form on this page.

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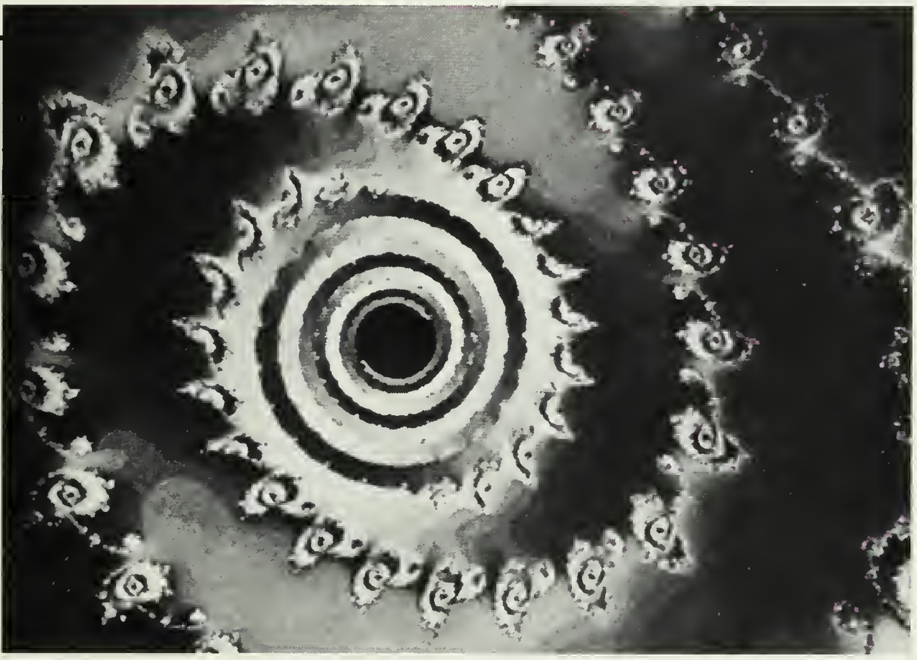
access

NCSA newsletter
January - February 1988, Vol. 2 No. 1



The supercomputer-generated image of a "fractal" was created by University of Illinois doctoral student Brian Evans. A composer, Evans has created a work of music and video images derived from the same source—a set of mathematical equations. *See article on page 5.*

Industrial Partners Program

MOTOROLA JOINS INDUSTRIAL PARTNERS PROGRAM

Motorola, Inc., one of the world's leading manufacturers of electronic equipment, systems, and components, has joined the NCSA Industrial Partners Program, company and NCSA officials announced Dec. 21.

In a three-year, $3 million agreement, Motorola researchers and computer managers will receive training in advanced computing technologies and will conduct supercomputer-based research on projects of interest to the corporation.

Motorola, which last year had a record $5.89 billion in sales, is the fourth major corporation to join the program. On November 12, Eli Lilly and Company became a partner, preceded by Amoco Corporation in August 1987 and Eastman Kodak Company in August 1986.

Motorola produces two-way radios, pagers, cellular radio-telephones, and other forms of electronic communications systems; semiconductors; defense and aerospace electronics; automotive and industrial electronic equipment; and data communication and information processing and handling equipment for the worldwide marketplace.

NCSA Director Larry Smarr said the partnership was especially fitting because of the University of Illinois' tradition of semiconductor research, including work by Nobel laureate John Bardeen, co-inventor of the transistor, and several colleagues and students. Also, the university is the site of the National Science Foundation's Engineering Research Center for Compound Semiconductor Microelectronics.

"We are very excited about Motorola joining our industrial program because it has long shown worldwide leadership in the critical fields of electronics, computer chip manufacturing, and communications," Smarr said. "The complexity of modern electronic components has become so great that supercomputers are becoming necessary tools in the design cycle."

Mel Slater, Motorola's director of engineering computing aids, said, "The center's vision of the role of supercomputing as an integral part of an overall scientific and engineering computing environment is strongly endorsed by Motorola."

The agreement places NCSA in a "leadership position" in the national drive to link the best scientific minds in industry and universities with advanced computing technologies, according to John Stevenson, coordinator of the NCSA Industrial Partners Program.

— William Allen

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Center Activities

NEW NCSA POLICIES ON CLOSING CRAY PROJECTS

NCSA celebrates its second birthday this month. Growing pains have been few, but one of the hardest has been creating an environment in which a researcher can proceed with his or her work with little bureaucratic harassment. And while accomplishing this, the center must still be able to maintain some control over the amount of service units to be delivered and the time frame for their delivery. NCSA therefore has developed new procedures and utilities to close out projects with as much advance notice to the user as possible.

There are two occasions when a project might be closed:

- The service units (SUs) allocated have been depleted.
- The expiration date has been reached.

Allocation Depleted

Effective February 1, 1988, a login system banner will inform you when a project's allocation is 80 percent depleted. It is up to the principal investigator (PI) to apply for more service units if they will be necessary to complete the work in progress.

NCSA has built in additional service units for researchers by allowing access to a project until 110 percent has been used, at which point the bankpoints of the project will be set to zero. Users will still be able to log on to a project to use the free utilities available (such as to move or copy files) but it will not be possible to run jobs. A list of free utilities is available by entering the CRAY command `help free`.

The PI should contact Patricia Wenzel at the BITNET address: `wenzel@ncsavmsa` to let her know that he or she has applied for additional service units. If she is not notified of this within a month following usage reaching 110 percent, the project will be closed and users will no longer be able to log on to that project.

If a supplemental application is made and approved, bankpoints will be reset to 1/25th of the service units allocated.

Expiration Date Reached

Two months prior to an expiration date, a letter will be sent to the principal investigator with information on the status of the project (allocation and usage) and suggested ways for the PI to proceed. For instance, if a project has been depleted above the 80 percent point, it will be suggested that the PI apply for additional service units if they are needed to complete the work. If less than 80 percent has been depleted and the PI wants to continue to access this project, the PI should write to Wenzel justifying the need for an extension. In the past, the policy of the National Science Foundation has been to grant at least a six-month extension with a short letter of justification from the PI.

If no request is made within one month beyond the expiration date, the project will be turned off and no users will be able to log on to that project.

Comments or questions on this policy may be addressed to Patricia Wenzel at the BITNET address: `wenzel@ncsavmsa`.

— **Patricia Wenzel**

CUMULATIVE INDEXES AVAILABLE FOR 1987 ISSUES OF ACCESS AND DATA LINK

Now you can locate any of the articles in Volume 1 of the ***access*** and ***data link*** newsletters from the NCSA by checking their cumulative indexes for 1987. Mailed with this issue of ***access***, the indexes list all of the articles in each newsletter by topic so you can easily refer to subjects of interest to you. All issues (1 through 5) of each newsletter are indexed.

To obtain a copy of any article indexed, simply order the back issue of the newsletter in which the article originally appeared. To order a back issue, call NCSA at (217) 244-0072. In the first quarter of 1988 NCSA will be distributing the new *NCSA Technical Resources Catalog*, which you can use to order back issues.

ACADEMIC AFFILIATES TRAINING

NCSA will soon host two more weeks of intensive training for its academic affiliates. During these training sessions, an academic affiliate campus sends a representative to NCSA for a week to learn technical details about the center's supercomputing systems, workstation environment, software, and other resources, as well as the details of the NCSA Academic Affiliates Program. This person then acts as a local consultant for the users at the affiliate site.

The next session for new affiliate consultants will be held March 7-11 at the NCSA. Topics covered will include: the CRAY X-MP/48, CTSS, workstations, networking, supercomputing tools, code vectorization/optimization, NCSA policies, and the affiliates program. This session is called the Academic Affiliates Training Session Phase I.

A follow-up session for our current affiliate consultants who have already attended a Phase I session will be held February 15-19 at the NCSA. This is the Phase II session. Topics planned are: the CRAY architecture, code optimization/vectorization (more in-depth coverage than Phase I), the Alliant architecture, parallel processing, multitasking, the CRAY-2, and graphics. In addition, updates will be given on the range of programs currently underway and being planned at the NCSA.

These sessions also give affiliate consultants a chance to meet and interact with each other and with the NCSA staff. They also afford participants an opportunity to provide feedback to the NCSA about the program and other NCSA services and programs.

To register for one of these sessions, or for more information about the NCSA Academic Affiliates Program, contact Joseph Hardin at the BITNET address: `hardin@ncsavmsa`, or by phone at 217-244-0072.

PEER REVIEW BOARD MEETS IN PITTSBURGH

The joint PSC/NCSA Peer Review Board met in Pittsburgh on December 3. The board accepted, with regret, the resignations of Herbert Scarf, Sterling Professor of Economics, Yale University, and Andrew McCammon, Department of Chemistry, University of Houston. Ralph Roskies, Director of the Pittsburgh Supercomputing Center, will work with NCSA to fill the vacancies in these areas. In addition, the board will add a member in the area of materials science.

Ralph Roskies announced the appointment of a new board member, Ray Chin, NSF Program Director of Computational Mathematics, who will fill the vacancy in mathematics.

NCSA indicated to the board that the NCSA supercomputer is at the saturation point. As a result, the board has to be more rigorous in the review of proposals presented to them. Several proposals reviewed were granted partial allocations, and the applicants are being requested to present clearer justification for the amount of service units requested. The board is also asking some applicants whether they have considered other numerical methods and is suggesting possible alternatives.

The board granted allocations for each center as follows:

PSC	1706	of 3486 requested (49%)
NCSA	1223	of 2821 requested (43%)

The 1988 schedule of PRB meetings and deadlines for applying follow:

Meeting: Tuesday, March 8, 1988
Deadline for Applications:
February 1, 1988
Meeting: Thursday, June 16, 1988
Deadline for Applications:
May 16, 1988

An announcement of a new National Science Foundation (NSF) allocation policy will be sent to users at all supercomputing centers by the NSF in the near future. NCSA will report on the new policy and procedures in the next edition of ***access***.

— Patricia Wenzel

VISITORS AT NCSA

Colleen Barton. Dec. 13, 1987-Jan. 8, 1988 from Stanford University. Area of research: geophysics.

Ken Bishop. Sept. 27, 1987-Feb. 10, 1988 from University of Kansas. Area of research: petroleum engineering.

Galen Gisler. Jan. 11-15 from Los Alamos National Laboratory. Area of research: astrophysics.

Philip E. Hardee. Jan. 20-26 from University of Alabama-Tuscaloosa. Area of research: astrophysics.

Scott King. Jan. 4-6 from California Institute of Technology. Area of research: geodynamics.

Gilbert Mains. Jan. 4-6 from Oklahoma State University. Area of research: chemistry.

Larry Tesler. Dec. 13, 1987-Jan. 8, 1988 from Apple Computer, Inc.

JACK WORLTON SPEAKS TO NCSA

Jack Worlton (left) and NCSA Director Larry Smarr (right).

Jack Worlton, a well-known name in the supercomputing arena, spent a week at the NCSA meeting with representatives from each area of the center. During his stay, he gave four lectures at the NCSA Interdisciplinary Research Center. The lectures were entitled:

- Trends in the Scientific Computing Environment
- Technology Forecasting for Supercomputers
- Toward a Science of Parallel Processing
- Supercomputers: A Market Analysis

The lectures were each approximately 1-1/2 hours in length and were well attended. NCSA staff and other attendees expressed very favorable comments regarding the lecture series.

Worlton is retired from Los Alamos National Laboratory, where he spent over 30 years in numerous management positions. He is now president of Worlton and Associates, a consulting firm specializing in supercomputing.

He was a member of the National Research Council's Committee on Supercomputer Evaluation and a member of the National Science Foundation's Technical Review Group for Supercomputer Centers. He was a member of NASA's Technical Review Committee for the Aerodynamic Simulator and has served on numerous supercomputer committees for the U.S. Department of Energy.

Worlton has been a national lecturer for the Association for Computing Machinery in the United States and has presented invited lectures worldwide.

—**Alan Craig**

WHITE BECOMES INDUSTRIAL PARTNER LIAISON

Larry White, assistant director of NCSA Industrial Partners Program.

As part of the growth and continued success of the NCSA Industrial Partners Program, Larry White (formerly workstation development manager) has assumed the position of assistant director, NCSA Industrial Partners Program. He is responsible for the internal program development of the operational aspects of this program. In his new position, White will be the partners' chief liaison and interface within the NCSA.

The Workstation Development Group, which White built and managed during the past two years, now reports to Lex Lane, NCSA manager of software. This group will continue to locate, develop, and distribute software that improves scientists' abilities to access and use the NCSA's supercomputer resources.

Networking

OBTAINING ACCESS TO NSFNET

If you want to access the NCSA facilities via NSFnet but you are only connected to SDSCnet, you may gain access by acquiring an account on the San Diego Supercomputer Center Gateway VAX. If you need such an account, send the following information:

- name
- phone number
- address
- electronic mail address
- short explanation of why you need access to NSFnet

to Paul Love at the following address:

Mr. Paul Love
Manager, Peripheral-Communications
San Diego Supercomputer Center
P.O. Box 85608
San Diego, CA 92138

You can also send electronic mail to:

`loveep@sdsc` (BITNET address)
`loveep@sds.sdsc.edu` (ARPA Internet address)

Focus

University of Illinois doctoral student Brian Evans.

MUSIC AND VIDEO SHARE EQUALLY IN EVANS' ART

In what may be the first use of a supercomputer for pure fine art, a University of Illinois composer has created a work of music and video images derived from the same source–a set of mathematical equations.

With the help of a National Science Foundation grant and NCSA's CRAY X-MP/48 supercomputer, Brian Evans, a University of Illinois doctoral student in music, composed a musical score and color movie of abstract geometric patterns. The work is call "Marie Sets."

In addition to its supercomputing aspect, "Marie Sets" is unique in its integration of music and visuals derived from the same source, according to Evans. This is in contrast to such classical animations as the Disney movie *Fantasia* and modern rock videos, in which the music already exists and the animation is created to match it.

"We have always had music placed in service to film and would find it unusual to watch a film without a musical score," Evans said. "The interest in my work is in combining the two so that they are, as much as is possible, equal partners in the work." The particular algorithm he used for generating "Marie Sets" describes abstract geometric shapes known as fractals.

After imposing certain aesthetic controls on the process, Evans ran the algorithms through a program on the CRAY X-MP/48. The numbers that resulted from the computation were translated into color images for a video screen and music for a stereo sound system.

The final work consists of a nine-minute videotape in five movements, or "collections." Exotic, spiraling fractal shapes constantly evolve, while computer-generated grand piano and vibraphone engage in a pleasant, intriguing duet void of the dissonance that characterizes much of experimental or "new" music.

Unlike other images produced at NCSA by "renaissance teams" of scientists, artists, and computer professionals, "Marie Sets" was created without a specific scientific focus. Instead, its purpose was aesthetic, Evans said. "Until now, the high artist has not really had an opportunity to get to these powerful tools," he said. "I feel privileged and fortunate to get access to them."

Evans decried the suggestion by some art critics that using computer technology to create art is dehumanizing. "Using a computer to do art is no different from using a hammer and chisel," he said. "It's just a tool for doing artwork. This specific kind of artwork could not exist without a powerful computer."

Evans, who in December finished his doctorate in music composition with a minor in computer science, spent eight months developing the algorithm and computer program with which he created "Marie Sets." He then improvised with these tools, exploring hundreds of variations of the aesthetic controls in search of sounds and images. "This part of the process was done exactly as if I were to sit down and write a composition for a string quartet," he said. He compared the various supercomputer runs to a composer's striking a chord on a piano, contemplating its aesthetic value for a moment before deciding whether to incorporate it into a composition, and then moving on to strike the next chord. "This is where the advantage in using a supercomputer comes in," he said. "The CRAY computer gives me a much more useful turnaround time than other computers. From a practical standpoint, if a composer has to wait 15 to 20 minutes to hear and decide if he likes the note, that is a very limited environment for doing creative work." For example, a computation of Evans' images and music that would take about four days on a typical state-of-the-art personal computer only requires about a minute on the supercomputer.

Evans first presented "Marie Sets" at the 1987 International Computer Music Conference, held at the University of Illinois at Urbana-Champaign in August. He is confident that his artwork represents only a modest beginning for computer music-animation.

"In mapping the 'Marie Set' algorithm to graphic and musical materials, I have used simple and direct methods of translation," he said. "As more sophisticated mappings are investigated, frighteningly endless possibilities of artistic expression suggest themselves."

—William Allen

Profiles

GETTING DOWN TO BUSINESS AT NCSA

Business Office Staff. Standing from left to right—Harriett Weatherford, Sandy Long, Barbara Sykes. Seated from left to right—Katie Henry, Kay Weidner, Tish Lehigh.

The Business Office is one of the stars of NCSA. When an organization grows as fast as NCSA, it takes a talented and dedicated group of people to keep up with the amount of financial and contractual paperwork generated by that growth.

At NCSA, the Business Office is the one department that must interact with every group concerning financial needs for equipment, staffing, and program requests. More specifically, the business office staff budgets NCSA's financial allocations and monitors spending.

Within that mission, the Business Office is charged with several key responsibilities. One is to handle all financial and personnel matters for NCSA. This includes projecting budgetary needs as well as taking care of purchases and payroll. Other responsibilities include making sure that all of NCSA's dealings concord with University of Illinois regulations and ensuring that research funds are spent properly.

Harriett Weatherford, NCSA's Associate Director for Finance and Administration, is heavily involved in another of the business office's crucial roles—budgeting financial support for funding requests. She and her staff work with NCSA's research scientists and other personnel to make sure their research proposals contain accurate funding requests.

In preparing the budget for a proposal, the researcher provides a skeleton budget that usually includes only the basic staff and equipment needs unique to the research. Then the business office staff works with the researcher to prepare a complete budget request, including travel, training, supplies, and benefits. The final budget is formatted for the receiving agency, approved by the University, and sent to the funding agency. If approved, the business office staff must monitor the research project's account to ensure that the funds are spent according to the approved budget.

The Business Office carries the burden of tracking how all grant funds are spent. This tracking is put to good use when it comes time to report to the various agencies who support NCSA. "We're continually justifying our existence to our funding agencies," Weatherford said.

For example, the NCSA administrative and research staff prepares annual and quarterly reports for the National Science Foundation so that NSF can review and renew the present funding appropriations to NCSA projects. The Business Office's accounts must show that grant money has been used properly.

The Business Office's role of ensuring that all NCSA's activities satisfy University of Illinois policy is also crucial. NCSA is classified as a special unit under the U of I Graduate College. NCSA's accounting and bill-paying functions are carried out through the University, according to regulations set by the State of Illinois. This means that all of NCSA's spending policies and contracts must be approved by the University and adhere to its policy.

Describing the day-to-day functions performed by the staff of the Business Office is difficult. Barbara Sykes, Assistant Director for Business Affairs, said the group is still trying to get to the point where they have a typical day. Much of their time is spent arranging purchase orders for equipment and coordinating payments for vendors. To help keep up with an increasing demand for accurate accounting and inventory information on a need-to-know basis, the group uses IBM workstations to retrieve information directly from the University's administrative database.

Sykes said that one of the intricate assignments handled regularly by her staff is software contracts. These are sometimes complex because NCSA deals with both the academic and commercial levels of supercomputer applications. This happens because NCSA is a nonprofit organization and its industrial partners are not. Vendors sometimes charge different rates for profit and nonprofit uses of the same software.

Like NCSA's other departments, the Business Office has grown rapidly—from one person to a staff of more than five full-time people. When NCSA opened in February 1985, its business functions were carried out by Jan Wehmer, Assistant to the Director, while a search was conducted for a permanent business director. In October of that year Harriett Weatherford was hired for the position, and the Business Office was born.

—Phil Hattwick

NEW USER TRAINING SESSIONS SCHEDULED

NCSA will be offering two-day intensive training sessions for users of the NCSA CRAY X-MP/48. The new user sessions will include the necessary information for getting started with the NCSA systems. Laboratory exercises are included. Topics will include: the CTSS operating system, using the DDT debugger, job control, code optimization and vectorization, some of the software packages available at NCSA, and other topics necessary for getting started on the NCSA CRAY computer. Enrollment is limited.

The schedule for the sessions is as follows:

January 25, 26	New User Training
February 4, 5	New User Training
February 29, March 1	Topics to be announced
March 28, 29	Topics to be announced
April 25, 26	New User Training

If you would like to extend your visit at NCSA beyond the training program dates, contact Patricia Wenzel at (217) 244-0072 regarding the NCSA Visitors Program.

To register, contact Tammie Hildreth at (217) 244-8306. For more information about the training program, contact Alan Craig at (217) 244-1988, or send BITNET mail to: `training@ncsavmsa`.

NCSA'S STUDENTS—A VALUABLE RESOURCE

Who are nine of the youngest regular users of the CRAY? They are NCSA's student consultants.

The first student consultant was hired in the spring of 1986, and NCSA now has nine student consultants charged with the task of learning the business of NCSA's user services and dealing with those users alongside the regular consultants.

Dave McWilliams, manager of the consultants, said the students work 10 to 20 hours a week. Up to eight of those consultants' hours are spent in the consulting office once the student is ready to handle user requests. The work includes reading and writing tapes for users, making videotapes from user data, and working on individual programming projects. They are also charged with assisting the regular consultants by monitoring and answering user requests and questions in the consulting office. About half the work done in the consulting office is performed by student consultants.

Although many of those hired as student consultants already have FORTRAN programming experience, McWilliams said most of the training is on the job, especially when it comes to dealing with the CRAY. "They learn a lot from sitting in on user training," he said. The program benefits many of the students in more than one way. Not only do the students become capable of working on the CRAY, but three student consultants have gone on to become full-time NCSA staff under the User Services group.

Seven of the nine consultants are graduate students. Their names and area of study are: James Joseph, electrical engineering; Chip Mayse, computer science; Satheesh Menon, mechanical engineering; Todd Saunders, electrical engineering; Jean Scarpelli, computer science; Dan Simkins, mathematics; and Lou Wicker, atmospheric science.

NCSA also has two undergraduate student consultants: Mark Champion, electrical engineering, and Steve Morley, mathematics/computer science.

—**Phil Hattwick**

Software

MINPACK PACKAGE AVAILABLE

The MINPACK package is now available on the NCSA CRAY computer. MINPACK is a package of FORTRAN subprograms for the numerical solution of systems of nonlinear equations and nonlinear least squares problems. See ***data link*** for details.

UNIX UTILITIES AVAILABLE ON THE CRAY X-MP/48

NCSA has acquired many UNIX utilities from SDSC that were originally developed at MFE from AT&T SystemV sources. Twelve utilities are available in public file space. See ***data link*** for details.

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New Accounts/Users	217-244-0074 `uadmin@ncsavmsa` (BITNET) `uadmin@ncsaa.ncsa.uiuc.edu` (Internet)
Visitors Program	217-244-0074 `uadmin@ncsavmsa` (BITNET) `uadmin@ncsaa.ncsa.uiuc.edu` (Internet)
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VAX 800 Numbers	800 533-7051 (baud 300/1200/2400) 800 533-3559 (baud 9600)
CRAY IP Address	`ncsad.ncsa.uiuc.edu` (128.174.10.48)
Front-end VAX BITNET Address	*`user@ncsavmsa`*
Front-end VAX IP Address	`ncsaa.ncsa.uiuc.edu` (128.174.5.100) `ncsab.ncsa.uiuc.edu` (128.174.5.101)
NSFnet Problems (NSF Network Service Center)	617-873-3400 `nnsc@nnsc.nsf.net`
ARPANET Problems (SRI-Network Information Center)	800-235-3155 415-859-3695 `nic@sri-nic.arpa`

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data link Vol. 2 No. 1 Preview

CHANGING YOUR CRAY PASSWORD

This article describes a new utility on the CTSS operating system for the CRAY supercomputer called `passwd`, which allows you to change your CRAY login password.

FORTRAN SUBROUTINE NAME CONFLICTS

FORTRAN subroutines can be found in your source code, binary object modules, and subroutine libraries. When the same subroutine name is used in more than one of these places, it may not be obvious to you that your program loads the correct routine. This article outlines how to avoid subroutine naming conflicts.

MINPACK PACKAGE AVAILABLE

The MINPACK package is now available on the NCSA CRAY X-MP/48. MINPACK is a package of FORTRAN subprograms for the numerical solution of systems of nonlinear equations and nonlinear least squares problems.

NCSA ACCESS FROM X.25 INTERFACED PUBLIC DATA NETWORKS

Through an international numbering plan for Public Data Networks (PDNs), it is possible to access the NCSA front-end VAX from a number of networks throughout the world. This article describes how to compose the correct international number for your point of origin.

UNIX UTILITIES AVAILABLE ON THE CRAY X-MP/48

The NCSA has acquired many UNIX utilities from the San Diego Supercomputing Center. There are currently 12 utilities available in public file space on the CRAY X-MP/48. This article tells you what they are and what they do.

data link is a collection of technical articles for NCSA computer users. If you do not receive ***data link***, but are interested in one of the above articles, call NCSA at 217-244-0072 to get a copy of the article. If you want to receive ***data link*** on a regular basis, fill out the subscription form on this page.

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University of Illinois at Urbana-Champaign

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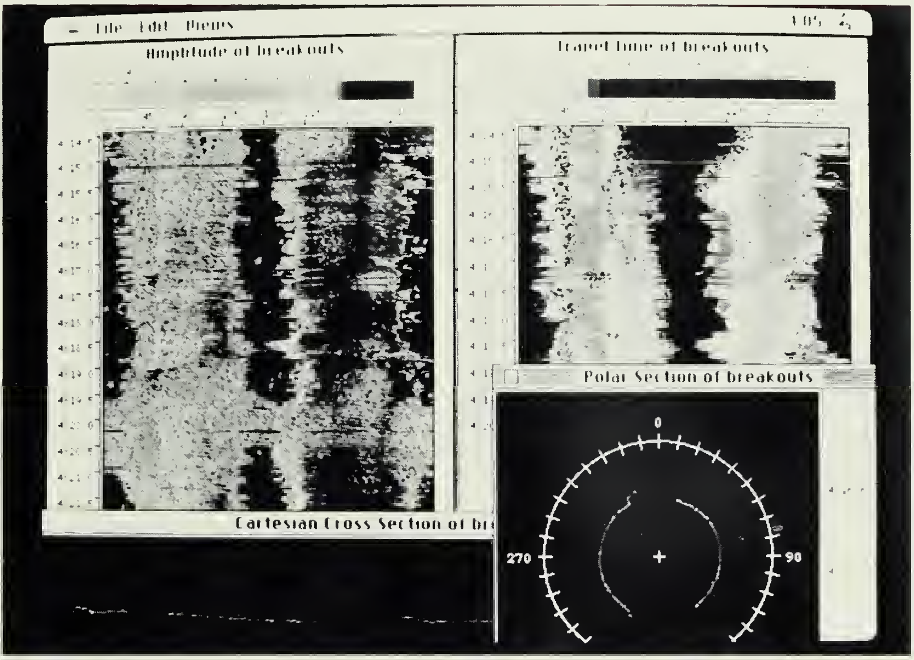
NCSA newsletter
March - April 1988, Vol. 2 No. 2

Visitors Program

LARRY TESLER AND COLLEEN BARTON VISIT NCSA



Larry Tesler's and Colleen Barton's Macintosh II program displays a 360° split image of the inside of a drillhole from a geothermal well in New York state. The dark vertical features displayed are "breakouts" caused by in situ stresses in the earth's crust.

Apple Computer, Inc. encourages its employees to take "Apple Sabbaticals" periodically. These sabbaticals enable Apple's staff to try something different for some weeks or months. Larry Tesler, Apple's vice president for advanced technology, is interested in developing scientific applications for the Macintosh II and in using his wife's geophysics research as a test case. He chose to take his sabbatical at NCSA to do this. He and his wife arrived at NCSA on December 13, 1987 and departed on January 8, 1988.

Larry Tesler has been deeply involved in microcomputing for a very long time. He worked at the Xerox Palo Alto Research Center (PARC) during the 1970s and was one of the architects of the Smalltalk computer language. While at PARC Mr. Tesler gave a tour of the facility to Steve Jobs, who was then at Apple Computer. During this tour Mr. Tesler demonstrated for the first time to Mr. Jobs the window-mouse-menu interfaces that have become the standard on Apple's Macintosh computers.

Mr. Tesler's wife, Colleen Barton, will receive her Ph.D. in geophysics at Stanford University this summer. Her thesis research involves analyzing data generated by sensors dropped inside very deep boreholes. The sensors spin as they are lowered into the hole, scanning the borehole interior with pulsed sound waves. The echo interval and strength gives information on the shape and composition of the borehole.

The data from the boreholes were converted and loaded onto NCSA Macintosh II computers. Larry Tesler and Colleen Barton wrote a custom program during their NCSA visit to display and analyze her data. Their program is similar in some respects to NCSA's Mac II image processing program, ImageTool, but it has many refinements specific to Ms. Barton's data. For example, the borehole data are cylindrical, so a cross section of her data produces a circle.

The borehole data traveled many routes during the couple's visit. Besides being displayed by their custom program and by ImageTool, the data were also given to NCSA's scientific visualization team. Stefen Fangmeier, NCSA visualization specialist, is currently working with Ms. Barton to produce a high quality videotape of her data, using very sophisticated 3D visualization techniques.

Both Larry Tesler and Colleen Barton were very impressed with the staff and facilities at NCSA. This visit also gave us at NCSA an opportunity to share personally our vision of scientific computing with high-level Apple staff.

— Brand Fortner

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Editor's Apology

On page 4 of the last issue we switched identities of these two gentlemen. We regret the error.

To set the record straight, NCSA Director Larry Smarr is on the left and supercomputing consultant Jack Worlton is on the right.

Center Activities

APPLE COMPUTER PRESENTS GIFT TO NCSA

Larry Tesler, Apple Computer, Inc.'s vice president of advanced technology, and Barbara Bowen, also of Apple, have announced an unrestricted gift to NCSA of $240,000 and 12 Macintosh II computers "to assist NCSA in enhancing the excellence of its research program in the visualization of scientific data and to enable the support of outstanding student researchers." It is expected that these funds and equipment will be used to support the development of scientific software.

Mr. Tesler was favorably impressed with the quality of the NCSA software projects and staff during his recent visits (see story on page 1). He was particularly interested in NCSA's image processing program, ImageTool.

ImageTool for the Macintosh II, produced by the NCSA Workstation Development Group, has just been released. The Mac II version is based on a program for the Sun Workstation by NCSA research scientist Mike Norman and research programmer Carol Song. The Workstation Development Group, managed by Martin Knapp-Cordes, currently includes two full-time employees and five student employees.

NCSA expects to use part of the additional funds to support software development in the RIVERS project (Research in Interactive Visualization EnviRonmentS), led by NCSA adjunct professor Robert Haber. Possible projects include advanced image processing tools; real-time graphics environments; and interactive, distributed simulation.

The remaining funds may be used by NCSA's Applications Software Group, managed by Lex Lane. Macintosh II projects of this group include further development of ImageTool, graphics foundations, graphics post-processors, distributed graphics environments, and HyperCard.

Much information will be shared between the RIVERS team and the Workstation Development Group. RIVERS concentrates on advanced research and prototype software, while the Workstation Development Group concentrates on deliverable software for both local and remote users. The workstation team's software will be readily available to NCSA users and to others, such as Apple Computer, Inc. All of these projects will be overseen by NCSA's recently created Computational Science Workbench Committee.

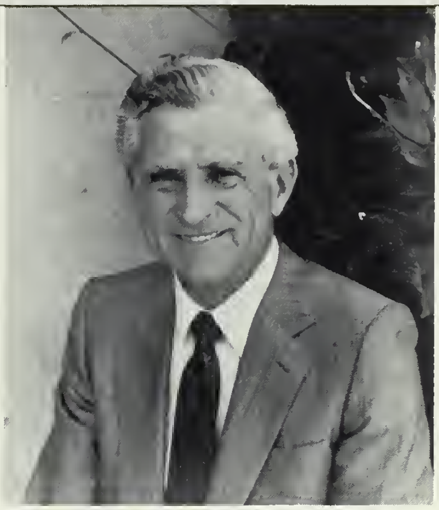
In announcing the unrestricted gift Mr. Tesler added, "American research universities have played a primary role in contributing to the technological excellence and industrial competitiveness of U.S. industry. The University of Illinois' National Center for Supercomputing Applications is a world-class research center. The development of intellectual capital in conjunction with NCSA research activities benefits U.S. industry in both direct and indirect ways. The development of talented and skilled researchers contributes a great deal to both the academic and corporate communities."

Apple is committed to making the Macintosh II a serious contender in the scientific workstation marketplace. This gift will help NCSA achieve its research mission to provide the best computational solutions to our users, whether they are using supercomputers or Macintosh IIs.

— **Brand Fortner**

THE NCSA TECHNICAL RESOURCES CATALOG IS HERE

The new *NCSA Technical Resources Catalog* accompanies this issue of ***access*** and replaces the *User Documentation Catalog* issued in July 1987. This catalog provides a comprehensive view of NCSA user documentation, video training materials, and software. It also includes complete ordering information. The next update of the *NCSA Technical Resources Catalog* will be mailed in July.



Dr. Gene M. Amdahl

THE FUTURE OF SUPERCOMPUTERS

On March 22, Dr. Gene M. Amdahl—a distinguished computer designer, author, inventor, and entrepreneur—will present a seminar at NCSA entitled "Limits of Expectation," in which he will discuss the future of supercomputers.

For nearly 15 years Dr. Amdahl worked at IBM. In 1965 he was named an IBM Fellow. During his five-year fellowship, Dr. Amdahl helped found and was named director of IBM's Advanced Computing Systems Laboratory in Menlo Park.

Leaving IBM in 1970, Dr. Amdahl formed and operated Amdahl Corporation. In 1980 he founded yet another company, Trilogy Systems Corporation, to design and market large, high-performance computer systems.

Dr. Amdahl is holder and coholder of many patents on such developments as recognition of recorded intelligence, analog-to-digital conversion device, message display and transmission system, stored logic computer, large-scale shifter, memory protection system, storage protection system, and the IBM System/360.

For further information regarding Dr. Amdahl's seminar, please contact Peggy Olsen at (217) 244-6832.

NEW ALLOCATION POLICY FROM NATIONAL SCIENCE FOUNDATION

The National Science Foundation (NSF) has announced a change in the way allocations will be made at the supercomputing centers. In the future, proposals received directly by NSF will be reviewed and then forwarded to the appropriate center board with a recommendation on the allocation. It will be up to the local boards to make the allocations.

NCSA has taken this opportunity to review its allocation procedures and policies as well. Following are the new procedures, policies, and criteria.

Requesting an Allocation

Allocation requests may be sent either to NSF or to NCSA. Requests sent to NSF will be reviewed and, if appropriate, forwarded with a recommendation on the allocation to the joint Peer Review Board (PRB) of NCSA and Pittsburgh Computing Center (PSC). ***All*** allocations for 51 or more service units (SUs) will be made by the PRB. Allocations for 50 or fewer SUs will be made by the NCSA Small Allocation Committee.

Startup requests for 5 or fewer SUs may be granted by an administrative review dependent on availability of machine time. Researchers at academic affiliate institutions (see list of current NCSA academic affiliates on page 15) should request startup grants at their own institutions.

Requests for more than 5 SUs will be sent to two reviewers who are NCSA principal investigators. In addition, those requests for 51 or more SUs will be reviewed and allocated at the quarterly PRB meeting (March, June, September, and December). Proposals must be received by the first of the month preceding the meeting (February 1, May 1, August 1, and November 1) to allow adequate time for review.

Multiyear proposals will be considered. Allocations will be granted each year based on available supercomputer time and a progress report review.

Extending a Project

Projects have a lifetime of one year, except for grants made to accommodate college classes. These grants are valid only for the semester or quarter in which the class meets.

Requests for supplemental allocations require a report of progress to date and justification for the additional SUs. A copy of any preprint or reprint based on this work should be sent to NCSA and should include an acknowledgment of the NCSA facilities.

Requests for an extension of the expiration date of the account should include justification for the extension as well as plans for completing the project. **One extension of six months may be granted. Only 25 percent of the unused SUs will carry forward.**

Judgment Criteria

Proposals are now judged according to the five criteria listed below. Criteria a. through d. are quoted from the *NSF Manual #10*, Proposal and Award Manual, section 121.2.

"Four criteria for the selection of research projects by the National Science Foundation are listed below, together with the elements that constitute each criterion.

"a. Criterion 1—Research performance competence. This criterion relates to the capability of the investigator(s), the technical soundness of the proposed approach, and the adequacy of the institutional resources available, and the proposer's recent research performance.

"b. Criterion 2—Intrinsic merit of the research. This criterion is used to assess the likelihood that the research will lead to new discoveries or fundamental advances within its field of science and engineering, or have substantial impact on progress in that field or in other scientific and engineering fields.

"c. Criterion 3—Utility or relevance of the research. This criterion is used to assess the likelihood that the research can contribute to the achievement of a goal that is extrinsic or in addition to that of the research field itself, and thereby serve as the basis for new or improved technology or assist in the solution of societal problems.

"d. Criterion 4—Effect of the research on the infrastructure of science and engineering. This criterion relates to the potential of the proposed research to contribute to better understanding or improvement of the quality, distribution, or effectiveness of the Nation's scientific and engineering research, education, and human resources base."

In addition, NCSA includes the following criterion:

e. Criterion 5—The adequacy of the proposal's numerical techniques as related to the proposed problem and the degree to which these techniques have been optimized for the appropriate supercomputer.

— Patricia Wenzel

CONSULTING OFFICE EXPANDS HOURS

Effective February 22, the NCSA Consulting Office is staffed from 8:00 a.m. to 5:00 p.m. CST.

You can reach the Consulting Office by calling (217) 244-1144 or contacting `consult@ncsavmsa` (BITNET address) or `consult@ncsaa.ncsa.uiuc.edu` (Internet address).

1987 ANNUAL SCIENCE REPORT AVAILABLE

The *NCSA Annual Science Report to the National Science Foundation for 1987* is being distributed to principal investigators and other interested people. If you would like to receive a copy, please write to: Office of Central Administration, NCSA, 605 East Springfield, Champaign, IL 61820.

This 348-page report includes brief summaries of more than 200 of the over 600 research projects allocated at NCSA in 1987. It also lists NCSA projects for 1987 as well as the nearly 550 citations received by December 1, 1987. These citations are of publications, videotapes, and presentations relating to work being done on the CRAY X-MP system at NCSA. The citations list will be updated quarterly. To receive an updated list of citations, please write to the NCSA Office of Central Administration.

LOOKING AHEAD—WORKSTATIONS FOR PROTEIN MOLECULE RESEARCH

Protein researchers and computer experts should join to conceive and develop an advanced computing environment dedicated to research on protein molecules, says Larry Smarr, director of NCSA.

Such "protein workstations" would accelerate research on how the molecules fold into complex biological structures, a key area of investigation for scientists in universities, industry, and government.

New knowledge about protein folding could affect a wide range of human concerns. For example, it could improve the understanding of disease and the design of new antibiotics and other drugs.

"A protein workstation would put at scientists' fingertips a combination of technologies already used to great advantage in such fields as astrophysics, atmospheric science, and mechanics," Dr. Smarr said February 14 in Boston at the annual meeting of the American Association for the Advancement of Science.

"The process by which proteins fold themselves from a linear sequence of amino acids into a complex three-dimensional structure is one of the great unsolved problems on the frontiers of biology," he said. "Supercomputing will play a critical role in both the theoretical understanding and practical implementation of this process."

In nature, the genetic code prescribes particular sequences of amino acids that make up particular proteins. A major goal of supercomputer use in this area is to calculate the shape of the protein molecule that results when a given sequence of amino acids is constructed and folds.

"The molecule could fold itself into an enormously large number of possible three-dimensional configurations," Dr. Smarr said. "Therefore, it is likely that the supercomputer will be used hand in hand with insights gained in laboratory experiment and theoretical expectations."

The protein workstation envisioned by Dr. Smarr would take advantage of several recent technological innovations used by scientists in other fields who have conducted research at the Illinois supercomputing center. These innovations include:

- an increase in raw computing power. Due in large part to parallel processing, this power is opening new approaches to research problems. Because supercomputers can handle increasingly large simulations of the physical processes found in nature, increasingly bold and imaginative questions can be posed and attacked.

- access to distributed sets of computers via high-speed networks. The computers provide varied levels of calculational power, as well as a wide range of information through specialized databases.

- visualization. This technique converts the millions of numbers generated by supercomputer simulations into color movies. These sophisticated animations help scientists gain new insight into specific phenomena in ways computer printouts cannot.

- multiple-window workstations. Sitting at a personal computer workstation in his or her office, a scientist can work simultaneously on different aspects of the same project by bringing up several "windows" on the screen. Each window itself represents a screen; for example, while a supercomputer run is monitored in one window, the results of the previous run can be plotted graphically in a second window, and the text for a scientific paper could be written in a third.

Dr. Smarr invited major researchers in protein studies to collaborate with researchers at NCSA in defining the functional requirements of a protein workstation. He called for the formation of a national task force to move the idea from concept to reality.

"The final software will be made available to the national community," he said. "Such standard software, coupled with a nationally networked research community, should greatly accelerate the rate of scientific progress on this key research problem."

He said he expects several scientists at the University of Illinois to become involved with the protein workstation effort, including those associated with the university's Prokaryotic Genome Analysis Center and Arnold O. and Mabel M. Beckman Institute for Advanced Science and Technology, and with NCSA's industrial partners.

— William Allen

SCIENTIFIC VISUALIZATION PROGRAM ESTABLISHES REVIEW BOARD

NCSA announces that the Scientific Visualization Program has established its Visualization Review Board (VRB). Craig Upson, former NCSA graphics research scientist who has recently joined Stellar Computers, Inc., serves as chairman of the board. The VRB also includes Michael Keeler, former manager of computer graphics at the San Diego Supercomputer Center who is now at Ardent Computers, and Dick Weinberg, professor of computer science at the University of Southern California. A fourth board member is yet to be named. Board members have been chosen for their expertise in scientific visualization and familiarity with the NCSA program.

At their first meeting, an all-day session held February 12 at NCSA, the board members discussed criteria for evaluation, toured the facility, met with program personnel, and reviewed proposals.

The VRB confers once a month by telephone to evaluate program applications and once a year at NCSA to allocate resources of the Scientific Visualization Program. In a team-oriented, human-intensive approach, the program integrates the scientist with computer graphics experts and sophisticated hardware and software to model and animate scientific data in three dimensions.

Criteria for review of applications to the VRB include:

- the introduction of visualization techniques to new scientific disciplines.
- the possible development of new algorithms, rendering techniques, illumination models, object–database generation, animation techniques, geometric primitives, usable code to be shared with other people, and the enhancements of conventional techniques to handle very large databases and complicated object topology.
- the visual aesthetics inherent in the project.
- the contribution to both scientific visualization and the computational sciences.
- the level to which the project will make the science more comprehensible to the scientist's peers and to laypeople.

The VRB does not determine the project's scientific merit. The only requirement is that a project has been reviewed previously by the National Science Foundation, NCSA, or another grant-awarding agency.

When the services offered by the Scientific Visualization Program are inappropriate for a proposed project, the board refers the applying scientist to other NCSA personnel and software that can better serve him or her.

Scientists interested in applying to the Scientific Visualization Program to visualize their three-dimensional data should send their names and addresses to `johnston@ncsavmsa` (BITNET address) or `rjohnston@ncsa.uiuc.edu` (ARPA-Internet address).

— Veronica Johnston

INTERNATIONAL CONFERENCE ON COMPUTATIONAL PHYSICS TO BE HELD IN BEIJING

On June 1–5, 1988, the International Conference on Computational Physics will be held in Beijing, China. The conference is being sponsored and organized by the Institute of Applied Physics and Computational Mathematics (IAPCM, Beijing) and Drexel University (Drexel, Philadelphia) in cooperation with World Scientific Publications (WSP, Singapore), China Association for Science and Technology (CAST, Beijing), and the National Center for Supercomputing Applications (NCSA, Champaign).

This conference will provide an opportunity for scientists and engineers in computational physics and computer science to meet one another, to exchange new techniques, and to discuss future prospects of algorithms and architectures of supercomputers. Participants will use slides, movies, and video presentations to demonstrate the use of graphics and imaging in research. New computing equipment and workstations will be exhibited.

Cochairing this conference are Deyun Li of IAPCM and Da Hsuan Feng of Drexel University. Among those serving on the Organizing Committee are NCSA Director Larry Smarr and Richard Isaacson of the National Science Foundation, who spent last year as a visiting research scientist at NCSA. The Advisory Committee for this meeting is Akito Arima, Nengkuan Chen, Kang Feng, John Gage, Bai-Lin Hao, Zuqia Huang, Neal Lane, Tsung Dao Lee, Kenneth Wilson, Peisu Xia, Yulin Zhou, and Fenggan Zhuang.

Invited speakers include:

Robert Ewald	Cray Research, Inc.
Steven Christensen	National Center for Supercomputing Applications
Bai-Lin Hao	Institute for Theoretical Physics, Beijing
Steven Koonin	California Institute of Technology
Gregory Mcrae	Carnegie-Mellon University
Robert Sugar	University of California–Santa Barbara
Craig Upson	Stellar Computers, Inc.
Michel Vallieres	Drexel University
Paul Woodward	University of Minnesota
Peisu Xia	Institute of Computing Technology, Beijing
Yulin Zhou	Institute of Applied Physics and Computational Mathematics, Beijing

APPLE DONATES MAC II COMPUTERS FOR PUBLIC USE

Bud Colligan, higher education marketing manager for Apple Computer, Inc, announced the donation of 15 Macintosh II computers to NCSA to be used in public areas. Eight of the new systems are now located in the Macintosh classroom, and seven more are available to NCSA's visitors in the visitors' carrels. These Macintosh IIs are top-of-the-line, with 80 MB hard disks, 5 MB of memory, and A/UX, when available. A/UX is Apple's version of UNIX for the Macintosh II. The systems are replacing the existing Macintosh Plus systems that have been available in NCSA's public areas.

Those Macintosh Plus systems have been installed recently in a separate, permanent training facility in rooms 171–173 of the Interdisciplinary Research Center. In the past, training programs (such as those for the NCSA Academic Affiliates) "borrowed" Macintoshes from staff desks and required lengthy setup. This permanent facility means that hands-on training classes are much easier to arrange and much less susceptible to network disruptions.

The upgrade of our public Macintosh workstations puts the best possible Macintosh hardware and software into the hands of our users. For example, our visitors can now use the new ImageTool software from NCSA on their workstations for color display of their two-dimensional datasets—something not possible on Macintosh Plus computers.

This donation is one of a series from Apple Computer in the last two years. The company has been exceptionally supportive of NCSA in its mission to provide the best possible hardware and software tools for the computational science community.

Larry Smarr, director of NCSA, is very excited about the Macintosh IIs at NCSA: "The Mac II has the potential to become a major 'port of entry' for remote supercomputer users throughout the country. We are eager to work with Apple and our users to develop software to tie together the distributed computing environment."

— **Brand Fortner**

TRAINING SESSIONS SCHEDULED

NCSA offers two-day intensive training sessions for users—particularly new users—of NCSA's CRAY computer system. These user training sessions provide the necessary information for getting started with the NCSA systems. Laboratory exercises are part of the training sessions. Topics include the CTSS operating system, using the DDT debugger, job control, code optimization and vectorization, some software packages available at NCSA, and other topics necessary for getting started on the NCSA CRAY computer. Enrollment is limited. The upcoming training schedule is:

March 28, 29	User Training
April 25, 26	User Training
May 26, 27	User Training
June 6–17	NCSA 1988 Summer Institute
June 27, 28	User Training

If you would like to extend your visit at NCSA beyond the training program dates, contact Patricia Wenzel at (217) 244-0072 regarding the NCSA Visitors Program.

To register for a training session, contact Tammie Hildreth at (217) 244-8306. For more information about the training program, contact Alan Craig at (217) 244-1988, or send BITNET mail to: `training@ncsavmsa`

PC HAPPENINGS

IBM has recently upgraded NCSA's two IBM PC/RTs as part of the ongoing IBM/NCSA Workstation Joint Study. Under this agreement, IBM placed $500,000 worth of equipment and software in the NCSA Interdisciplinary Research Center in the fall of 1985. In the spring of 1986 NCSA received two IBM PC/RT Model 25s from IBM.

The IBM PC/RT is a Reduced Instruction Set Computer (RISC) workstation. IBM's standard operating system offered on the RT is AIX. AIX is a System V-based implementation of UNIX. The RT is based on a dual bus architecture with an IBM PC/AT compatible 16-bit peripheral bus and a local, high-speed bus to link the processor, memory, and optional floating point adapter (FPA).

NCSA's RTs were each initially equipped with Advanced Monochrome Displays, 3 MB of memory, FPAs, and AIX software. In 1987 IBM announced the 100 series of the IBM PC/RT as well as an upgrade for owners of the earlier RT models. Now upgraded to Model 125s, NCSA's RTs are each equipped with an Advanced Processor Card, 4 MB of 100 nanosecond interleaved memory, an Advanced FPA, a Baseband (Ethernet) adapter card, and two 70 MB ESDI (enhanced storage device interface) disks. These workstations are being upgraded to 8 MB by IBM.

IBM upgraded one RT to a dual monochrome display system with the addition of an Extended Monochrome Display which supports a display resolution of 1024 x 768. The monochrome display for the other RT is being augmented by an IBM Megapel Display Adapter subsystem. The subsystem is comprised of a 19-inch color monitor and a 1024 x 1024 pixel, eight-plane (256-color) display adapter. Along with software upgrades to support the new hardware, IBM is donating additional graphics software, compilers, and the X-Windows system for use on the RTs.

IBM has announced an August release date for a version of AIX for the PS/2 Model 80. The PS/2 Model 80 is based on the Intel 80386 microprocessor. IBM has also announced Network File System (NFS) support for AIX on both workstations, also to be available in August.

IBM provided the following performance statistics for the PC/RT model 100 series:

	Standard Hardware	Optional FPA
Dhrystones	6500	—
Whetstones *	810K	1600K
Whetstones **	700K	1400K
Linpack FLOPS **	80K	300K

* single precision
** double precision

— **Mark Johnson**

SUPERCOMPUTING SUPPORTS RESERVOIR SIMULATION RESEARCH

Introduction

Professor Kenneth A. Bishop is a member of the graduate faculty in the Department of Chemical and Petroleum Engineering at The University of Kansas. His research activities include a program that deals with the mathematical description and simulation of the transient flow of fluids in petroleum reservoirs and groundwater aquifers. Currently on sabbatical leave from the university, Professor Bishop carried on his research as a long-term visitor at NCSA from September 1987 until February 1988, when he joined the NCSA staff as a consultant. In August he will return to his duties at The University of Kansas.

Dr. Bishop serves as the campus coordinator for the NCSA Academic Affiliates Program at his university. He has been active in the development and use of the MIDnet regional network and in the establishment of the infrastructure for supporting and monitoring supercomputing activities at The University of Kansas. The goal of these activities is to establish telescience as a viable means of carrying on computationally intensive research at locations remote from supercomputer centers.

This article is based on material presented during a seminar entitled "Network Access to Supercomputing Resources with Applications in Reservoir Simulation," given at NCSA in February 1988.

Background

The ability to sustain life and civilization as we know it depends on optimal management of a few critical resources. Among these resources fresh water (important for both irrigation of semiarid regions and direct life support) and petroleum (important as a source of both energy and raw materials in our carbon-hydrogen-based society) share a common characteristic. The principal storage environment for both resources is in the interstices of the rock that makes up aquifers and petroleum reservoirs. This shared trait forms the basis for a research program at The University of Kansas.

For an aquifer, optimal management implies balancing the withdrawal and recharge rates over time and locale. For petroleum reservoirs, the husbanding of a finite resource is implied. Management strategies for producing water from aquifers and oil and gas from petroleum reservoirs imply answers to questions regarding:

- drilling of wells: How many should be drilled and where should they be located?
- production policy: In what mode (production or injection) and at what rate should they be operated?
- recovery technology: For oil, what secondary and/or tertiary recovery technique is appropriate?

The answers to these questions rest upon economics, engineering technology, and an understanding of the chemistry and thermodynamics of the reservoir fluids and of the porous media that form the reservoir fabric. Understanding the physics associated with the flow of fluid through the porous media is equally crucial. Among the techniques that help us understand the physics is a special combination of transient pressure testing with reservoir performance simulation. As proven reserves steadily decline, contemporary economic forces are creating a need for ever more powerful, yet cost-effective, technology for predicting reservoir performance, thereby enabling more effective reservoir management.

The goal of the research program at The University of Kansas, which I codirect with Dr. G. W. Swift, is the improvement of the body of technology that supports the analytical test, normal operation, and optimal management activities that must be addressed during the life cycle of an aquifer or a petroleum reservoir.

The program involves both field tests and laboratory experiments. It also involves both physical and mathematical modeling of a fluid-filled reservoir. Its products include a unified body of transient-pressure-test-analysis technology for drawdown and buildup tests, as well as phenomenologically specific treatments of the Klinkenberg effect, non-Darcy flow, and well-bore storage and damage effects. Computation requirements in support of the various elements of the program are intense and growing.

The challenge to the research program generated by the growth of its computing requirements can be illustrated by an example. In 1982, a single run of a parameter identification code was terminated after it consumed university computing resources in excess of the level required to support the undergraduate curriculum of the Department of Chemical and Petroleum Engineering for one month. The computation ultimately required more than 30 CPU hours using a 2 megaflop machine. Recognition that this particular computation dealt with a problem whose size and complexity represented only average scientific and technical interest triggered an odyssey in search of computing power that has led to NCSA.

The Current Project

The project undertaken during my current visit to the NCSA involves extensive modification of a reservoir simulation code to be used in conjunction with a natural-language-prompted simulation manager (GRIP). The goal of the project is establishment of the feasibility of "telescience" as a mechanism for computationally intensive research at the university. The implementation involves use of MIDnet and NOVAnet as the means by which the existing program at The University of Kansas and the Interdisciplinary Research Center program at NCSA are tied to form a supercritical mass for conducting research in reservoir analysis and management. The goal will be achieved when the following two specific objectives of the current project are completed.

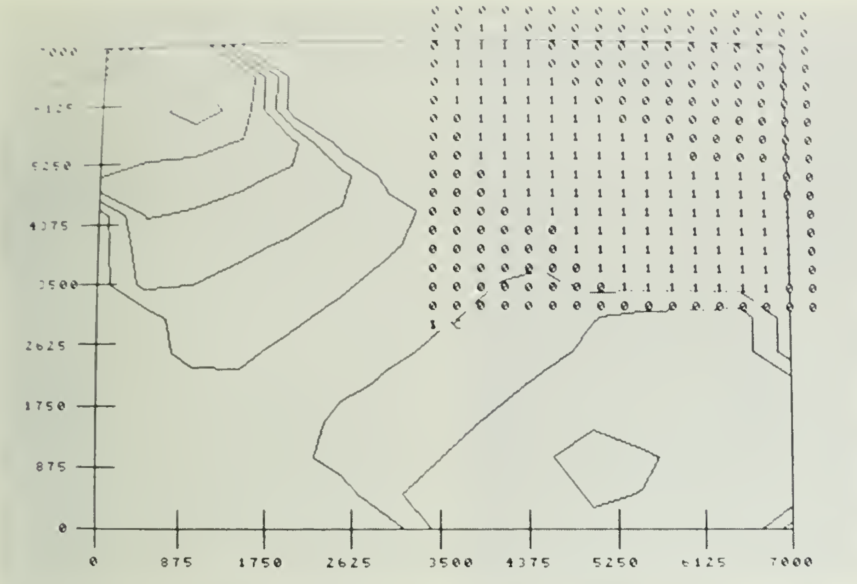


Figure 1. Isopotential Plot of Pressure

- Comparative execution times of the reservoir simulation code for problems of various "sizes" will be obtained. Three cases will be timed:
  - the Harris 1200, which is available at Kansas (base case).
  - the CRAY X-MP system running unoptimized code.
  - the CRAY X-MP system running optimized code.

  Meeting this objective will establish and document the adequacy of support for the current requirement, as well as a two-year growth estimate.

- The capability to undertake a larger project in which pre- and post-simulation activities are optimally distributed among the elements of the computing array is to be established. These activities include problem definition, parameter assignment, scenario management, output graphics display, and display management. The cases to be studied include:
  - accomplishing computational tasks using a computer of less than "super" capabilities. There is no network involvement (base case).
  - accomplishing all computational tasks on the supercompute. The responsibilities of the remote workstation are trivial. The combination of MIDnet and NOVAnet provides the communication bandwidths appropriate to transmission of user directives and output from graphics display drivers, respectively.
  - accomplishing reservoir simulation using the supercomputer. All pre- and post-simulation activities are accomplished using a powerful workstation in a remote location. The combination of MIDnet and NOVAnet provides the communication bandwidths appropriate to transmission of the simulation results as well as those of the pre-simulation.

Reservoir Simulation Methodology

"Conservation of mass" equations, written for each phase or constituent of the reservoir fluid contained in a volume element located in the porous media, generate a set of simultaneous partial differential equations. These equations relate the rate of change of mass of the constituent contained in the element, as a function of time, to the instantaneous mass fluxes of that constituent which cross the element's boundaries.

Inclusion of descriptive expressions for mass flux (Darcy's law) and thermodynamic equations of state for the constituents permit us to relate physically measurable quantities such as pressure or hydrostatic head to the independent variables (three space dimensions plus time) and the system driving functions (sink/source terms). Very simplistic models give rise to the classic diffusion equation. In these simplistic models:

- rock properties (permeability and porosity) are considered isotropic, homogeneous, and constant.
- flow is considered exclusively diffusive.
- reservoir fluid is considered incompressible.

Introducing realism in any of these areas, as well as including technologically important features (well bore anomalies, fracture treatments, or injection of another fluid complicate the mathematical model of the reservoir significantly.

It is very common to employ mathematical models in which:

- the potential (typically pressure, head, water saturation, or concentration) appears nonlinearly.
- the variation of the properties with location, flux direction, and potential precludes algebraic collection of terms in the model.
- the nature and position of boundary conditions vary with time.
- the source/sink terms are complicated functions of time.

These complications force solution of numerical approximations rather than of the nonlinear partial differential equations. Finite element and finite difference approximations are commonly used. In either case, it is necessary to solve very large sets of simultaneous nonlinear algebraic equations at each time step.

Reservoir Simulation *continued on following page*

The results of a test made with 64x the spatial resolution used to produce Figure 1 are displayed in color raster form on the screen to which Dr. Bishop is pointing.

***Reservoir Simulation** continued from previous page*

Project Methodology

The code used in the project undertaken during my visit to NCSA simulates the movement of water in a confined, isotropic, homogeneous aquifer under the influence of a tailorable, multiple-well pumping program. The model consists of a single (essentially linear) constant coefficient parabolic partial differential equation in two space dimensions, plus time. The finite difference numerical approximation consists of a set of mildly nonlinear simultaneous algebraic equations that, when represented in vector matrix notation, involves a pentadiagonal coefficient matrix that must be eliminated at each time step.

The Alternating Direction Implicit Procedure is employed in order to replace the elimination of an n^2 by n^2 matrix at each time step with $2n$ eliminations of an n by n tridiagonal matrix at each time step. The Thomas technique is used to upper-triangularize and unzip the augmented coefficient matrix. The principal mechanisms available for controlling the problem "size" involve increasing the resolution of the grid employed in the finite difference representation of the model and increasing the temporal resolution of the simulation. Since the solution techniques being used are unconditionally stable and convergent, the problem "size" can be manipulated essentially at will.

Early Results

The initial phases of the study involved porting (to the CRAY X-MP system) and validation of the code we are using. This process was made quite convenient by the existence of the code implemented for, and running on, the Harris H1200 at The University of Kansas. The simulator can be accessed via the local network, MIDnet, and the X.25 campus network at Kansas. Because problems of arbitrary complexity and configuration may be set up using the problem-oriented simulation manager (GRIP), it is easy and convenient to create problems with which to test the code by means of pattern recognition applied to the resulting graphic output. The CRAY computer's implementation of those same problems must behave identically if the port was successful.

Figure 1 shows an example of the process. It is a contour plot of the pressures that exist at steady state when water is injected at the well located in the upper left-hand corner of the figure and removed (at the same rate) from the well located in the lower right-hand corner of the figure.

The test involves lack of movement of the isobars with increasing time once steady state has been achieved. The effect of the complicated geometry imposed on the problem is indicated by the shapes of the individual isobars. The array of zeros and ones superimposed on the upper right-hand corner of Figure 1 is a scaled mapping of the grid locations used to produce the isopotential plot. The injection well is located at node 4,4 (row, column), and the production well is located at node 14,12. The 1 indicates that a node is located in zone 1 (inside the reservoir); the 0 indicates that a node is located in zone 0 (outside the reservoir).

Parts of each of the two specific objectives of this project have been reached.

- Comparative execution times of the reservoir simulation code for problems of various sizes have been obtained for both the Harris 1200 (base case) and the CRAY X-MP system running unoptimized code.

- Computational tasks using a computer of less than "super" capabilities and with no network involvement (base case) have been accomplished.

Current activity focuses on:

- Accomplishing all computational tasks on the supercomputer. Specifically, the impact of the increased spatial resolution afforded by the CRAY X-MP system is being evaluated.

— Kenneth A. Bishop

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Hilst , R. W. and K. A. Bishop. "GRIP: A Problem-Oriented Language." *Computers and Chemical Engineering,* 5, no. 4, pp. 249-262, 1981.

USING THE CRAY X-MP SYSTEM TO CHANGE HISTORICAL RESEARCH

A professor of history and his colleagues are using NCSA's CRAY X-MP computer system to change historical research. A year from now historians will see the results of his groundbreaking study, the world's first automated record-linkage program run on a supercomputer.

Vernon Burton, professor of history at the University of Illinois at Urbana-Champaign, believes that supercomputers will vastly change how historians analyze the past and predict the future. He has devoted much of his career to experimenting with the power of computers as a historian's tool.

How Historians Met the Computer Age

In the early 1960s a few adventurous historians began to use computers for quantitative analysis. Some of their colleagues objected, saying that history's most important questions could not be quantified. Others suggested that the potential to discover and theorize history is limited only by a historian's imagination and available tools.

During the last three decades, quantitative analyses provided by computers have helped historians study complex questions once considered unthinkable. Historians have been learning to use this powerful tool, which makes possible studies involving huge stores of data, such as monitoring population demographics over long periods of time or tracing the flows of large populations. Information storage, retrieval, and manipulation is perhaps the greatest benefit of computers today for historical research. The enormous speed and storage capacity of the CRAY system make it especially valuable, as Dr. Burton has found out through his own experience.

In the mid-1970s Dr. Burton was one of Princeton University's first wave of graduate students to use computers in the study of history. Well versed in using both huge historical databases and handwritten census data from the Civil War era, he demonstrated the value of computers to the accurate understanding of history in his book, *In My Father's House and Many Mansions,* which was nominated for the Pulitzer Prize in 1985.

According to conventional wisdom, the existence of black matriarchies could be traced back to the days of slavery. According to this theory, female slaves headed black households before the Civil War and continued to do so after the Civil War. Using a historical database on a mainframe computer to study old Edgefield County in South Carolina, Dr. Burton disproved this long-held belief.

In the Civil War era Edgefield County sprawled across South Carolina, but today it has been broken into five counties. Earlier researchers could study only small population samples to deduce overall patterns. By using a computer to store countywide census data collected between 1850 and 1880, Dr. Burton was able to analyze the entire population of Edgefield County. His study of the whole population uncovered different demographic patterns for the hinterlands, small towns, and cities that had been lumped together in the small samples of previous scholars. His computer-based analysis demonstrated convincingly that the existence of a black matriarchy was a myth, not historical fact, and that wealth—more than race—influenced family structure among blacks and whites immediately after the Civil War.

Nominal Record Linkage on the Supercomputer

Despite the proven usefulness of computer analysis in historical research, Dr. Burton still faced limitations imposed by computer hardware. In particular, the limited speed and capacity of mainframe computers meant that Dr. Burton was repeatedly told to merge his databases after midnight because his procedures monopolized the system.

Then, in 1986, Vernon Burton heard Larry Smarr speak about NCSA and the CRAY supercomputer. Dr. Smarr described software that enabled a researcher to work on different databases simultaneously, then integrate the databases using a mouse or joystick. Dr. Burton perceived that such software could be valuable to his ongoing research project, Nominal Record Linkage, which is the tracing

***Historical Record** continued on following page*

Dr. Vernon Burton at his workstation.

Historical Record continued from previous page

and linking of an entire population's progress through time. Nominal record linkage enables historians to study such topics as the geographic and economic mobility of American society.

Dr. Burton also recognized several benefits from using the CRAY X-MP system to run regional studies with nominal record linkage. These benefits are that the database can be large enough to store entire populations, computations can be run at high speeds for large sets of data, and demographic patterns from a database can be graphically displayed to detect net patterns.

As he explored opportunities for historical research on the supercomputer, Dr. Burton met a linguist, Atsushi Fudaka, who had already developed portable algorithms for nominal record linkage. When Mr. Fudaka joined Dr. Burton's research project, he added an interdisciplinary angle to the project.

Future Supercomputer Use by Historians

Once the development of nominal record linkage on the supercomputer has been completed and used in historical research, Dr. Burton anticipates that techniques of historical research will be modified and that many existing historical beliefs will be revised. He recently told fellow historians, "As the questions are refined by historians, we cannot be sure what might be important for future investigations. We may have argued for 'total history,' that is, the inclusion of all the people from the census or at least a stratified sample, but we have not really used all the variables in all the records that were available."

Community studies—the kind of historical research that will benefit most from nominal record linkage—have been popular for a long time, but large-scale community studies have not been attempted because of technical limitations. NCSA's CRAY X-MP computer system overcomes many of those limitations and is beginning to change how historical research is done.

Already graduate students have applied to do their research with Dr. Burton using nominal record linkage. One, Terence Finnegan, is at work studying lynching and patterns of lynching throughout the South in the 19th century. Other graduate research projects are still under consideration.

The ultimate value of using supercomputers for historical research may lie in the kinds of studies that will be possible for the first time. Vernon Burton looks from the past to the future when he suggests, "The supercomputer allows you to do some of the same types of research, but on a *regional*—perhaps someday even on a *national*—level."

— **Phil Hattwick**

VISITORS AT NCSA

Ken Bishop. Sept. 27, 1987–Feb. 15, 1988 from University of Kansas. Area of research: petroleum engineering.

Richard H. Durisen. Feb. 15–23 from Indiana University. Area of research: physics.

Charles Evans. Feb. 9–17 from California Institute of Technology. Area of research: astrophysics.

Sam Finn. Feb. 9–17 from Cornell University. Area of research: astrophysics.

Michael J. Foote. Mar. 9–11 from University of Chicago. Area of research: evolutionary biology.

Philip E. Hardee. Feb. 23–25 from University of Alabama at Tuscaloosa. Area of research: astrophysics.

Helga M. Leonhardt Hendricks. March 4–14 from The Leonhardt Language System, Inc. Area of research: language application.

Jacob Klerman. Feb. 22–29 from University of Chicago. Area of research: economics.

Leonard F. Register. Feb. 29–Mar 11 from North Carolina State University. Area of research: quantum transport.

Dwight Woolard. Feb. 29–Mar. 4 from North Carolina State University. Area of research: electrical and computer engineering.

Andrew Zachary. Mar. 9–11 from University of Chicago. Area of research: astronomy and astrophysics.

Industrial Partners Program

A NEW INDUSTRIAL PROGRAM—ASSOCIATE PARTNERS

Many corporations have expressed a desire to participate in NCSA's Industrial Partners Program but are not yet ready for the commitment NCSA requires of its full industrial partners. To meet the needs of these corporations, NCSA announced in January the availability of associate partnerships in its industrial program.

Corporations can become associate partners with NCSA for a minimum period of one year. They will receive training in the use and management of supercomputing resources as well as priority distribution of NCSA publications. Researchers from the corporation will visit NCSA to use the corporation's allocation of supercomputer resources.

The NCSA Industrial Partners Program is under the direction of John Stevenson, corporate relations officer. For more information on this program please contact his office at (217) 244-0474.

— **Larry White**

Focus

RESEARCHING ANCIENT LITERATURE WITH A COMPUTER

The IBYCUS Scholarly Computer is flanked by David Bright (left) and David Sansone (right).

A new computer system that allows instant access to all of Greek literature is opening new avenues of investigation for University of Illinois scholars in the humanities and for computer researchers who aim to develop "scholars' workstations" for many disciplines.

The IBYCUS Scholarly Computer provides, in machine-readable form, the full body of Greek literature, from Homer to the sixth century, "opening the way to hitherto impossible options for research," says Dr. David F. Bright, chair of the Department of the Classics.

The IBYCUS computer, named for an ancient poet, is "a little like having all of Greek literature on the shelf, all at your fingertips," Dr. Bright said. That means classicists, philosophers, linguists, and other scholars can complete in a few minutes research projects that once would have taken a lifetime or were even impossible.

The scholars' workstations effort is a joint project of the NCSA and the Department of the Classics; it is funded by these two units and by the College of Liberal Arts and Sciences and the School of Humanities. The joint project grew out of talks between Dr. Smarr and faculty members in the School of Humanities on how NCSA could bring advanced computing technologies to humanists, Dr. Bright said. These led to discussions about creating a new kind of scholars' workstation.

California computer engineer and classicist David Packard designed the IBYCUS system. It provides access to a 62-million-word text base of Greek literature prepared at the University of California at Irvine for the "Thesaurus Linguae Graecae." The text base is contained on a CD-ROM, a compact laser disk that stores massive databases.

The disk also contains a sizable amount of Latin and Coptic text and the Hebrew Bible. Future versions of the disk will include larger databases. Dr. Bright said the implications are enormous for linguistic research, literary analysis, historical questions—"the list is nearly endless."

"The impact will be felt not only in faculty research, but in the method and very subject matter of graduate seminars, dissertations, and other projects," he said. "Because it will also provide important information in the development of more advanced scholars' workstations of applicability to a broad range of humanists, it should be the vanguard of revolution in methods and areas of research across the humanities and elsewhere. In all of this, the University of Illinois stands to gain international notice."

While UIUC humanists are busy finding ways to use the IBYCUS system, researchers from NCSA will study its use and explore ways of giving general computer workstations similar capabilities. Of particular interest is developing CD-ROM technology for information storage.

"We are keen to get an early test of how people interact with such a massive database on a local computer," said Larry Smarr, director of NCSA. "If the effort in the humanities is successful, we hope that some faculty may want to develop their own CD-ROMs for specialized areas such as a particular language or author." Such compact disks might contain all of Nietzche's or Cicero's writing, the entire body of classical Latin, or all of medieval literature, including Old French and Anglo-Saxon.

In addition to providing rapid access to the entire surviving body of Greek literature, the IBYCUS system can tie in with Macintosh computers, which most faculty members in the department have. Information can be copied directly into their personal research files.

"One of the great plusses of the system is it's just very easy to use," said classics professor Dr. David Sansone, who only began using computers last year. Dr. Sansone is researching the text of Plutarch. He simply types into the computer a string of Greek letters, and the IBYCUS system searches the database for all occurrences of the string in Plutarch's works, a search that lasts less than one minute.

"Plutarch is one of those authors who hasn't been worked on as much as he should have been, particularly because the corpus is so large," Dr. Sansone said. "In the past, scholars

Researching *continued on following page*

Researching continued from previous page

have relied on their memories for retrieving passages from various parts of the corpus. Now we can call up parallel passages with great ease."

What impact the system will have on how humanities scholars do their work five years from now is difficult to predict, but the system puts them "at the beginning of a whole new phase of research methods," Dr. Bright said.

The Illinois IBYCUS system is one of only about a dozen in universities nationwide. Considering other computer facilities on campus, such as links to computer networks and the availability of personal computers to individual faculty members and graduate students, "it's fair to say our equipment is unsurpassed. We are in a position to take a leading stance in computer-assisted research in the humanities," Dr. Bright said.

Currently, faculty members in the classics, comparative literature, history, linguistics, philosophy, and speech communication departments are interested in using the system. Use is expected to increase as more scholars discover the IBYCUS system and as researchers enlarge the repertoire of issues they can address individually, he said.

— William Allen

Networking

NORTHWESTNET OUTREACH

Oregon State University hosted a NorthwestNet User Services Training Workshop on their campus in Corvallis, Oregon on January 11–14, 1988.

NorthwestNet comprises a number of schools in the Northwest region of the United States that have installed a 56 KB regional network to interconnect these schools and to provide each school with a path to the NSFnet backbone network. Members of NorthwestNet are:

- University of Alaska at Fairbanks
- University of Alaska at Anchorage
- University of Idaho
- Montana State University
- North Dakota Research Universities
- Oregon Graduate Center
- Oregon State University
- University of Oregon
- University of Washington
- Washington State University

Boeing Computer Services is the network manager and the Western Interstate Commission on Higher Education (WICHE) is the fiscal agent.

The recent training session, one of many planned by the NorthwestNet Training Committee, was intended to bring information about networking and the various supercomputer centers to the several NorthwestNet campuses. Each of the following supercomputer centers presented a two-hour overview of their respective centers, highlighting differences among the centers:

- Cornell National Supercomputer Facility (CNSF)
- John von Neumann National Supercomputer Center (JVNNSC)
- National Center for Supercomputing Applications (NCSA)
- National Magnetic Fusion Energy Computer Center (NMFECC)
- Pittsburgh Supercomputing Center (PSC)
- San Diego Supercomputer Center (SDSC)

The responses from the attendees were extremely positive and included such comments as: "Excellent use of time." "All supercomputer sites and all NorthwestNet nodes in attendance—great." "I gathered names and documentation that will be vital." "High-density information, little time wasted."

NCSA's staff are very interested in making similar outreach trips to other sites to share more information about supercomputing and related resources. If you are interested in having NCSA provide a presentation at one of your future sessions, please contact Alan Craig, NCSA training coordinator, at (217) 244-1988, or send BITNET mail to: `training@ncsavmsa`.

— Scott Lathrop

NCSA STARTUP MANUAL VERSION 2.0

The *NCSA Startup Manual* has been revised, and Version 2.0 is now available. The *Startup Manual* has five parts:

- *NCSA User's Guide* Version 2.0 describes NCSA facilities, computer hardware and software, and user support services. The *User's Guide* includes an appendix of sample sessions with the CRAY X-MP/48 and VAX computers, and provides a comprehensive index and glossary of terms.
- *CFTLIB Reference Manual* covers the most common CFT math library routines. It provides quick access to file assignment routines, utility routine interfaces, controllers and controllees, and other often-used routines. This manual is a subset of the *CFTLIB Manual.*
- *NCSALIB Reference Manual* is a summary of routines developed at NCSA at the request of users. It includes timing routines and bit-flipping routines.
- *DDT: Dynamic Debugging Tool Reference Manaul* summarizes DDT procedures and most common commands. It is a subset of the *DDT Reference Manual.*
- *NCSA Command Summary* is a quick reference booklet of commands and routines described throughout the *NCSA Startup Manual.*

The price of the *Startup Manual* is $25.00. To order, please write to: NCSA, Documentation Orders, 152 Computing Applications Building, 605 East Springfield Avenue, Champaign, IL 61820.

You will find complete ordering information in the *NCSA Technical Resources Catalog* that accompanies this issue of ***access.***

SUBSTANTIAL CHANGES FOR NCSA'S REMOTE USERS

One of the major issues facing users of any of the national supercomputer centers is the access to the facilities by remote users.

The intention of the National Science Foundation (NSF) is to provide a national network that enables researchers to collaborate remotely over high-speed networks and that provides researchers with easy access to the NSF supercomputer centers. This network, NSFnet, is operating across the country. NSFnet comprises both a backbone network, which links the five NSF centers and the National Center for Atmospheric Research (NCAR), as well as many state and regional networks, including NYSERnet, SURAnet, MIDnet, WESTnet, BARRnet, USAN, Merit, SESQUINET, and NorthwestNet.

The reality for many scientists is either that NSFnet does not effectively reach their offices or that they are unaware of the status of networking on their local campuses. This has prompted researchers to use alternate methods to access the NSF centers, including GTE Telenet and toll-free 800 numbers. These alternate access paths are expensive to operate, and NSF has no interest in paying for such access paths. The charges for 800 numbers at NCSA have become excessively high in recent months. Due to the recent cutback in our FY88 budget, free dial-up service has been removed.

We are asking all users to evaluate access paths and methods of working remotely. You should actively pursue a local connection to NSFnet. If you do not know the status of the network on your campus, we have provided an online lists of NCSA academic affiliate contacts and of NSFnet networking contacts. We urge you to contact these people to determine whether you can connect to your own local campus network or use a local dial-up access path to your local network node. The list of NCSA's Academic Affiliates, indexed by state or by institution can be viewed on the CRAY X-MP system by entering:

```
document view affiliates
```

and specifying a keyword using your institution or state. If your campus is not a member of the NCSA Academic Affiliates Program, you can see a list of NSFnet contacts on the CRAY X-MP system by entering:

```
document view nsfnet
```

and specifying a keyword using your institution or state. If you still cannot find anyone on your campus to help you, please send electronic mail to the NCSA Network Support Group at `network@ncsavmsa` (BITNET address), `network` (front-end VAX), or `network@ncsa.uiuc.edu` (ARPA-Internet address).

If you have no local access to NSFnet, you will need to use GTE Telenet at your own expense. Using Telenet at your own expense requires that you get a Telenet user ID from GTE Telenet. To obtain a Telenet user ID, send a letter to:

Jim Warmbir
Telenet Communications Corporation
2 Trans Am Plaza Drive, Suite 450
Oakbrook Terrace, IL 60181

In your letter you should mention that the master agreement is with the EDUNET/University of Illinois account. This statement is for administrative reference only; it does not in any way obligate the University of Illinois or NCSA to pay any charges that are not paid by you. The letter must be signed by you the user and must include the following information:

user's name
user's full billing address
user's phone number
preferred user ID or 3-20 characters

In less than two weeks you can obtain your Telenet User ID via U.S. mail.

If you need to transfer large amounts of data (< 300,000 bytes), we suggest that you transfer files over BITNET to the NCSA front-end VAX. You can also use magnetic tape. Tape formats are described in the *NCSA User's Guide* or are available from the NCSA consultants. Furthermore, the consultants will help you read and write your tapes to reduce the frustration of handling magnetic tapes.

If you are doing large amounts of editing, keep in mind that workstations provide a much more friendly environment for editing than does the CRAY X-MP computer system. We suggest that you use workstations to their full extent.

Please keep us informed of other ways in which we can help you to improve your networking access to NCSA.

— Scott Lathrop

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***Academic Affiliates** continued from previous page*

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Profile

APPLICATIONS SOFTWARE GROUP

The Applications Software Group. Back row from left to right—Lex Lane, Mark Johnson, Dave Heisterberg. Front row from left to right—Radha Nandkumar, Margaret Kubaitis, Beth Richardson.

NCSA's Applications Software Group is charged with installing, maintaining, and supporting vendor and other third-party software on the NCSA computer system. As basic software needs have been more nearly fulfilled, the Applications Software Group has been able to turn more attention to working with scientists to understand thoroughly the computational needs of research scientists and to work with vendors and other code developers to determine which applications serving those needs run best on the NCSA system. The applications group is designing an environment that meets the needs of NCSA's diverse community.

The work of the Applications Software Group will be increasingly influenced by NCSA's recently organized Software Selection and Oversight Committee (SSOC). Aiming to choose a balance of software so that NCSA's users in all fields of study are served, SSOC evaluates software requests and considers whether the software is already optimized for the supercomputer, whether a similar program is already running at NCSA, and whether adding the package will increase productivity among the scientific community.

Once software has been selected, the applications programmers arrange for the installation of packages, then optimize them for use on the supercomputer, benchmark the software, and implement whatever other changes are necessary to bring the package online for users. When needed, they draw on the expertise of key outside consultants.

Who Are The Applications Software Group?

Currently there are five programmers in the Applications Software Group. Dave Heisterberg focuses on the discipline of computational chemistry and works with semiempirical, ab initio, and molecular force field codes. Mark Johnson works with codes appropriate for continuum mechanics simulations. He is currently working on porting several finite element analysis codes to be used for structural analysis applications. In the past, Radha Nandkumar has supported DI-3000 and NCAR Graphics, and she recently installed MOVIE.BYU on the CRAY X-MP system (see this month's ***data link*** article). Her current efforts are devoted to the Astronomical Image Processing System (AIPS), which she is optimizing on the Alliant FX/8 parallel processing system. Beth Richardson is responsible for all numerical codes and math libraries on the CRAY computer system. Margaret Kubaitis tests codes and works on numerical library licensing and installation. Lex Lane, manager of systems and software, serves as acting manager of the group.

Evidence of the efforts of the Applications Group is the growing software list on page 18. This list was current as of March 4. In addition to installing and maintaining software packages, the applications group meets with researchers and vendors to learn what the supercomputer needs to be able to do and to learn what kinds of packages are available and being developed. For example, Mr. Heisterberg organized a computational chemistry workshop in December 1987 for a small, invited group of campus and remote researchers to learn what these chemists hoped would become available on the CRAY X-MP system.

What Does the Future Hold?

Yesterday's research code has become today's production application code in many notable cases. Much of the software on the NCSA system, while it has been carefully tuned to run on the supercomputer, was not designed and written specifically for the supercomputer.

The Applications Software Group looks forward to working with those who will be developing the next generation of supercomputer software—vendors and current users of the NCSA system. Fostering the development of this new generation of software on the supercomputer requires a rich applications development environment.

As the list of supercomputer applications software on the NCSA system

Applications continued on page 19

Software

APPLICATIONS SOFTWARE ON NCSA'S CRAY X-MP SYSTEM

This is a list of software currently available and in progress on the CRAY X-MP/48 system. It also lists oftware available to visitors on Interdisciplinary Research Center (IRC) workstations.

With a large and diverse user base, NCSA is always looking for new and more optimal software to meet program development and applications requirements of our users. We encourage you to suggest additional software packages. Your recommendations should, as much as possible, address NCSA's software evaluation criteria, which include user impact, new functions not supplied by existing software, the degree of optimization for CRAY machines, and a vendor contact.

Address correspondence to:

Lex Lane
NCSA
605 East Springfield Avenue
Champaign, IL 61820

Or send electronic mail to:

`13002@ncsavmsa`
(BITNET address)

Printed documentation can be purchased for most of the currently available software. See the *NCSA Technical Resources Catalog* that accompanies this issue of ***access.***

Available as of March 4, 1988

Chemistry Packages

AMPAC semiempirical molecular orbital analysis
CADPAC ab initio molecular orbital analysis
GAMESS ab initio molecular orbital analysis
GAUSSIAN86 ab initio molecular orbital analysis
HONDO ab initio molecular orbital analysis
MOPAC semiempirical molecular orbital analysis

Compilers

CFT CRI FORTRAN compiler
HCC vectorizing C compiler from LLNL

Engineering Packages

FIDAP fluid dynamics
PATRAN pre- and post-processor (IRC Sun)
SPICE electronic circuit simulation

Graphics Packages

DI-3000 Contouring device-independent vector graphics
DI-3000 device-independent vector graphics
IDL graphics package (IRC MicroVAX)
MOVIE.BYU 3D rendering and animation graphics
NCAR Graphics device-independent vector graphics

Mathematics Packages

ACM Algorithms general math
BCSLIB general math
CALMATH general math–high performance
CFTMATH general math
- SLATEC
- LINPACK
- EISPACK
- FISHPACK
- QUADPACK

ELLPACK elliptic boundary value
FFTLIB NCAR fast Fourier transform routines
FITPACK curve and surface fitting
IMSL general math
MINPACK nonlinear systems solver
NAGLIB general math
ODEPACK ordinary differential equations
PCGPAK sparse matrix solver, iterative method
PORT general math
S Plus AT&T statistics/graphics (IRC Sun)
SCILIB vector and matrix operations, FFTs
SMPAK sparse matrix solver, direct method
SSDLIN out of core linear systems solver
VECPACK vector and matrix operations, FFTs
XMP linear programming

Work in Progress

Chemistry Packages	Planned Availability
AMBER molecular mechanics and dynamic	4/88
CHARMM molecular mechanics and dynamics*	2Q88
CHEMX model analysis (IRC microVAX)	2Q88
GRADSCF ab initio molecular orbital analysis	2Q88
GROMOS molecular mechanics and dynamics	4/88
MACROMODEL molecular mechanics and dynamics(IRC microVAX)	2Q88
MM2 molecular mechanics and dynamics	2Q88

Compilers	
CFT77 CRI FORTRAN compiler	3Q88
PASCAL CRI PASCAL compiler	2Q88

Engineering Packages	
ABAQUS analysis	2Q88
DYNA2D dynamics	2Q88
MAZE 2D mesh generator	2Q88
NASTRAN structural analysis*	4/88
NIKE2D structural analysis	2Q88
ORION 2D post-processing/plotting	2Q88
PISCES electrical device simulation	2Q88
TOPAZ2D thermal analysis	2Q88

Graphics Packages	
IDL graphics package (IRCSun)	2Q88
PVI Graphmaker high-level interface to DI 3000	2Q88

Mathematics Packages	
BENCHLIB general	2Q88
ECMFFT fast fourier transform	2Q88
HARWELL general math	4/88
REDUCE symbolic manipulation	2Q88
SPSS statistics for social sciences	2Q88
TOEPLITZ Toeplitz form matrix–signal processing	2Q88

***User must pay for using this software**

Applications continued from page 17

becomes more nearly complete, the Applications Software Group will be devoting more attention to constructing the environment necessary to encourage the development of future generations of supercomputer software.

The key to all efforts—present and future—of the Applications Software Group is their commitment to providing an environment that meets the diverse needs of NCSA's users.

— Phil Hattwick

NOW AVAILABLE—IMAGETOOL FOR THE MACINTOSH II

The scientific visualization package, ImageTool, is now available for the Apple Macintosh II. A product of the NCSA Workstation Development Group, ImageTool for the Macintosh II is a direct descendant of the ImageTool prototype developed by Dr. Michael Norman and Carol Song for the Sun Workstation. The raster image files are byte streams with no demarcation between scan lines. ImageTool provides display and animation of color images as well as contour, 3D, and shaded data plots. It also features a variety of color palette manipulations. See this month's ***data link*** for more details about ImageTool for the Macintosh II.

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CRAY IP Address	`ncsad.ncsa.uiuc.edu` (128.174.10.48)
Front-end VAX BITNET Address	*`user@ncsavmsa`*
Front-end VAX IP Address	`ncsaa.ncsa.uiuc.edu` (128.174.5.100) `ncsab.ncsa.uiuc.edu` (128.174.5.101)
NSFnet Problems (NSF Network Service Center)	617-873-3400 `nnsc@nnsc.nsf.net`
ARPANET Problems (SRI-Network Information Center)	800-235-3155 415-859-3695 `nic@sri-nic.arpa`

NCSA's permanent training facility in the interdesciplinary Research Center. Apple's donation of 15 Macintosh II computers replaced the Macintosh Plus systems in the public classroom. The Macintosh Plus systems were then installed as part of this new training facility.
See Apple Donation article on page 7.

data link Preview Vol. 2 No. 2

ACCOUNT STATUS—QU UTILITY

One of the most frequently asked questions for NCSA consultants concern the status of time allocations on the NCSA CRAY X-MP computer. This article describes how to use the QU utility to retrieve cumulative usage information sorted by userid or by project.

ANALYZING APPLICATION PERFORMANCE—FLOWTRACE

This is the first of a series of articles explaining the tools that are available on the NCSA supercomputer system for analyzing the performance of your code. These tools will help you identify the bottlenecks of your codes so you can concentrate on them and try to optimize them.

ANALYZING APPLICATION PERFORMANCE—TIMER/TALLY

This article explains how to use `timer/tally`—a two-step timing procedure developed at Lawrence Livermore National Laboratory—in identifying portions of an application that can be optimized.

BATCH SCHEDULER USAGE

NCSA's CRAY X-MP computer system has a batch scheduler utility named `batch` which schedules long-running jobs. This article describes the process through which jobs are scheduled and the advantages of the `batch` utility.

BETTER FILE TRANSFERS WITH NMOVE

This article describes an improved file transfer process using `nmove` developed at NCSA. The new procedure eliminates most of the previous troubles associated with `nmove`, primarily through increased reliability.

FFTLIB—FAST FOURIER TRANSFORM SOFTWARE FOR THE CRAY X-MP SYSTEM

FFTLIB is an object library of vectorized multiple fast Fourier transform (FFT) routines callable from FORTRAN programs. This article discusses the features available and how to call those optimized routines.

JOBS STATUS—MONITORING CRAY JOBS IN THE FIVE SUFFIXES

The CTSS operating system on the CRAY X-MP computer allows users to run as many as five jobs in the five suffixes or process streams. This article introduces a new command, `js`, that allows users to check the status of jobs in all suffixes from a single suffix.

MOVIE.BYU—GRAPHICS SOFTWARE FOR THE CRAY X-MP COMPUTER SYSTEM

The MOVIE.BYU programs are now available on the CRAY X-MP computer system. This article explains the general purpose graphics utility and how to use it to manipulate data from mathematical, topological and architectural models.

NEW COLOR IMAGING PROGRAM—IMAGETOOL FOR THE MACINTOSH II

NCSA introduces Imagetool—a graphics package developed in house—that allows scientists to see data created on the CRAY X-MP computer by using color image display, animation, contour, 3D, and shaded data plots.

PRINT AND PLOT UTILITIES

This article describes the `print` utility on NCSA's CRAY X-MP computer system that allows users to request prints and plots.

TIMING COMPARISON OF DIRECT ACCESS AND RANDOM I/O

In general, I/O routines are a chief reason for slow code execution. This article summarizes timing comparisons of the standard FORTRAN unformatted `write` statement and the CFTLIB random I/O routine `wdisk`. It also compares the effects of using the solid-state storage device with those routines.

VECTORIZATION FOR CALCULATING THE MANDELBROT SET

This article shows, by way of example, how you can vectorize a seemingly nonvectorizable problem.

data link is a collection of technical articles for NCSA computer users. If you do not receive ***data link***, but are interested in one of the above articles, call NCSA at 217-244-0072 to get a copy of the article. If you want to receive ***data link*** on a regular basis, fill out the subscription form on this page.

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54 Computing Applications Building, 605 E. Springfield, Champaign, Illinois 61820.

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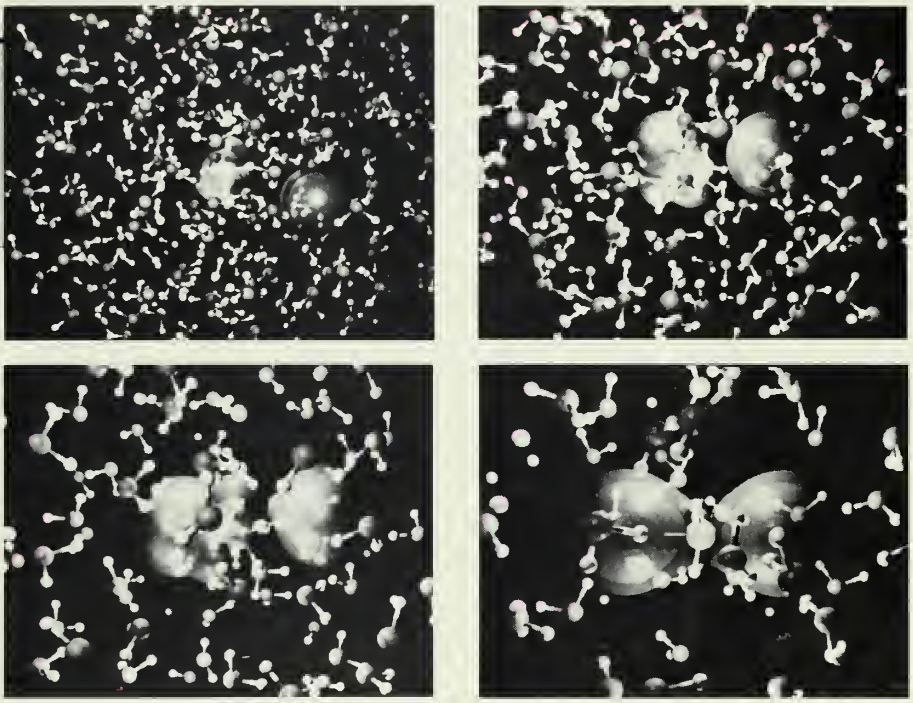
NCSA newsletter
May - June 1988, Vol. 2 No. 3

Scientific Visualization



Quantum Molecular Dynamics.

These images, as viewed with a zoom camera technique, show the reaction of chloride ion plus methyl chloride in water solution. *Photos by SMS*

Investigating Atom Exchanges

Paul Bash, Post-Doctoral Fellow in Theoretical Chemistry at Harvard University, is using the resources of the NCSA Scientific Visualization Program to demonstrate a method of studying molecules in condense phase (that is, in water or enzyme rather than in vacuum), to map out the movement of atoms and to relate this movement to what is known to occur in experiments.

Using data generated from a simulation run on a CRAY-2 supercomputer and created by Dr. Bash and Martin Field, also a Post-Doctoral Fellow in Chemistry at Harvard, this visualization shows the changing strength of the bonds between the atoms as well as the changing density of electrons of each atom in the reacting molecules. It is this density of electrons that changes and determines what happens during a chemical reaction.

During a four-day visit to NCSA in February, Paul Bash worked closely with the scientific visualization staff, particularly with software development supervisor Matthew Arrott and animators Michelle Mercer and Jeffery Yost. Within a week, this team created a draft videotape of the visualization, working with the simulation data, Wavefront Technologies Inc. software, and software specifically written for this project. The videotape demonstrates clearly that the behavior of a basic molecular reaction in vacuum is very different from the more nearly real-world reaction in water solution.

The first part of this project studies the replacement reaction of chloride ion (Cl^-) and methyl chloride (CH_3Cl) in both vacuum and water. Used as a refrigerant and local anesthetic, methyl chloride consists of a methyl group (one central carbon atom attached to three hydrogen atoms) and a chlorine atom. In methyl chloride's stable state, the methyl group swaps the chlorine atom on one side for a different chlorine atom on the other; the methyl group "exchanges" chlorine atoms because they have opposing charges. The methyl group remains intact during this exchange.

The first part of the videotape shows the calculation of this exchange in

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vacuum, in its gaseous state, unhampered by other molecules as it would in the real world. The sizes of the atoms are correct relative to each other, and the electronic bonds between the atoms are visualized by short rods joining bonds between the atoms.

The second part of the videotape (frames of which are shown here on page one) represents a much more complicated calculation that attempts to include the effect of water molecules on the exchange reaction as it actually occurs in solution. Each water molecule is two hydrogens attached to a large oxygen atom. These images show water molecules constantly bombarding methyl chloride molecules and preventing them from taking the straight-line movement that occurs in the vacuum sequence. Transparent surfaces have been used to add two levels of the electronic potential around the atoms, enabling you to see the long-distance effect of the electric charges on the surrounding space. As the moment of exchange nears, the videotape slows down the time evolution by a factor of 10 and zooms in on the bonds as they are breaking between the methyl group and the chlorine. There the bond breaks twice for each attachment to the chlorine atom because the methyl group cannot make a "clean getaway" from the chlorine while the group is surrounded by the crowd of pushing water molecules.

Both the simulation and the visualization of this study are complex. In terms of computer graphics, this visualization is a combination of dynamically generated, contour surfaces and more conventional dynamical "ball-and-stick" models of atoms and molecules. In the final rendering of any visualization, the geometry of the objects must be recalculated for each frame. In this project, some of the frames contain as many as 200,000 polygons—a complex visualization. Matthew Arrott said that while this project invented no new computer graphics techniques, it did use a very large database, which imposes constraints on conventional computer graphics. The project also effectively combined several different scientific computer graphics techniques.

The team of Matthew Arrott, Michelle Mercer, and Jeffery Yost created a visualization that went beyond the simple wire-frame graphics used by most chemists to study and describe their research. Jeff Yost explains that the services provided by the program are "labor-intensive, using ordinary, off-the-shelf software from the commercial world—but applied to science. Scientists typically use simple wire-frame drawings that are fast and easy to create but yield a minimum of information. Scientific visualization enables the scientist to see much, much more." Slides of wire-frame drawings of the molecules were used to indicate camera angle and rough shapes.

NCSA Director Larry Smarr termed the visualization of this research a "real breakthrough. This visualization takes the scientist down to the molecular level and allows one to intuitively do chemistry on an atom-by-atom basis."

Paul Bash said that it was important to visualize the "numbers" from his simulation. "[The visualization] verified my intuition of what was going on. I can't take a microscope at this level and take a snapshot, but visualization does it for me. I have much more insight."

— Veronica Johnston

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National Center for Supercomputing Applications; 605 East Springfield Avenue; Champaign, Illinois 61820

Coming Soon to a Planetarium Near You

Supercomputer-generated images of burgeoning thunderstorms, colliding stars, and vibrating biomolecules may soon light up the domes of planetariums across the nation.

In a pioneering collaborative project, specialists at NCSA and the William M. Staerkel Planetarium at nearby Parkland College plan to integrate aspects of the center's scientific visualization efforts into the planetarium environment. The joint project evolved out of discussions between Paul Magelli, president of Parkland, and Larry Smarr, director of NCSA. Dr. Magelli has appointed Parkland art instructor Jonathan Block as liaison with the center.

NCSA has pioneered ways for scientists to view complex scientific data in meaningful color images. Mathematical simulations of real-world problems on the center's CRAY X-MP/48 computer, which can perform 800 million arithmetic operations a second, produce mountains of data that are practically incomprehensible unless changed into visual form.

James Manning, left, and Carl Hoyer with the projected Earth. *Photo by UI News Bureau*

Benefits of the Project

"This project will give NCSA access to the very specialized presentation environment of the planetarium—a state-of-the-art facility that will further the center's visualization capabilities," said Carl Hoyer, resource consultant at NCSA. Mr. Hoyer and James Manning, director of the planetarium, are coordinating the effort.

The project could lead to scientific meetings that would use innovative computer graphics presentations to communicate more effectively among researchers in astronomy and a wide range of fields, Mr. Hoyer said. It also could lead to new educational presentations for students at all levels.

An especially challenging aim of the project is to make possible three-dimensional imaging on a full planetarium dome, Mr. Hoyer said. Such an accomplishment could advance supercomputer research on many subjects, from colliding stars to the molecular structure of diseases. Not only could simulated images then be viewed from the outside, they also could be "entered" and viewed from inside, leading to new insights.

State-of-the-Art Facilities

The Staerkel Planetarium features a Zeiss planetarium projector, automated auxiliary projectors, special effects equipment, an audience-surrounding sound system, and a 35-millimeter big-screen projection system.

The planetarium, which officially opened in October, offers a wide range of educational and cultural programs. Its regularly scheduled shows include "Odyssey," a journey through the solar system and into the depths of space and time, and "Visit to a Far Planet," about the Voyager space mission to Uranus and other planets.

The first projects planned for application to the planetarium are the slide show, "Renaissance Teams: A Convergence of Art and Science," which illustrates the efforts of artists and scientists to create scientific visualizations, and the "Etruscan Venus," a sculpture-like supercomputer visualization of complex geometric surfaces. This visualization was developed at NCSA by artist Donna Cox, mathematician George Francis, and graphics specialist Ray Idaszak. Mr. Hoyer said the center also will work with Chicago's Adler Planetarium and other planetariums around the nation to investigate new uses for computer graphics.

— William Allen

NCSA 1988 Summer Institute, June 6–17

The NCSA 1988 Summer Institute is being held at NCSA June 6–17. For information about the 1988 Summer Institute, enter

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help training institute
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on the NCSA VAX or CRAY computer. Look for an article on the NCSA 1988 Summer Institute in a future issue of ***access.***

RIVERS Project Underway at NCSA

An interdisciplinary group of NCSA research scientists, faculty, staff, and students have banded together to explore the possibilities of next-generation hardware and software systems for scientific supercomputing. The RIVERS (Research on Interactive Visual EnviRonmentS) project is a key component of the Computational Technologies Program within NCSA's in-house scientific research program. Apart from the acronym, the name RIVERS is intended to convey the notion of the massive streams of visual and numerical data that the group members envision flowing through their prototype computing environment.

The group is working closely with computer vendors to assemble advanced hardware systems for real-time visualization and animation, and for very high-speed (gigabaud) networking between supercomputers and visualization workstations. "After assembling the hardware systems, the real challenge will be putting together the software systems to allow scientists to make effective use of this impressive new generation of computer technology," said Robert Haber, NCSA Adjunct Professor of Supercomputing Applications and Group Leader of the RIVERS project.

The interdisciplinary nature of the project is reflected in the diverse backgrounds of the RIVERS members. These include NCSA research scientists, such as Michael Norman and Barbara Mihalas in computational astrophysics and Robert Wilhelmson in atmospheric science. University of Illinois at Urbana-Champaign (UIUC) faculty—Robert Haber (Civil Engineering and Theoretical & Applied Mechanics) and Donna Cox (Art and Design)—are also participants. NCSA research programmers Ray Idaszak, Polly Baker, and Clint Potter provide expertise in computer graphics and image processing. UIUC graduate students from the application disciplines and the Department of Computer Science round out the team.

Interactive scientific visualization is a key area for research and development in the RIVERS project. Through its Scientific Visualization Program, NCSA has become a national leader in the use of computer graphics and image processing in the analysis and interpretation of supercomputing data sets. Current methods involve a team of computer graphics experts, sophisticated graphics software, and a good deal of time to produce a video animation. The RIVERS group will be developing hardware and software systems for direct, interactive use by scientists to supplement the capabilities of the visualization program.

Advanced computer graphics hardware, capable of rendering complex three-dimensional images at rates of up to 30 frames per second, will be assembled in 1988. This will permit scientists to animate their results interactively in real time, without the laborious procedures needed for videotape animation. The ability to interactively alter the viewing parameters as the animation proceeds will substantially enhance the value of visualization for scientific discovery, prior to presentation and communication of results.

Beyond hardware performance, the lack of high-level software tools is a major obstacle to the widespread use of visualization in routine computational science and engineering. The RIVERS effort focuses on developing prototype software tools for interactive visualization. Portability between hardware from different vendors and between different hardware performance levels are important goals in this work. Emerging software standards and *de facto* standards, such as PHIGS+ and X.11/NeWS, will be used for portable tool development.

The work will be carried out in a multitier hardware environment, ranging from the Apple Macintosh II, through Silicon Graphics Iris systems and Sun-4 systems with Raster Technologies GX4000 rendering engines, to very high-end systems based on an Alliant FX/80 minisupercomputer.

Experience has shown that data transfer bottlenecks, rather than number crunching and computer graphics processing power, are often the limiting factor in the effective use of visualization in scientific computing. The RIVERS group is examining new mass storage technologies, such as disk striping, parallel transfer drives, and disk arrays, to deliver the large storage capacities and rapid effective transfer rates required for real-time animation. NCSA plans to install a 100 MBytes/sec network from Ultra Network Technologies later this year to support the transfer of massive data sets between supercomputers and remote visualization stations. The initial installation will connect the CRAY X-MP

Robert Haber, Group Leader of the RIVERS project. *Photo by SMS* supercomputer, two Alliant FX/80 minisupercomputers, and a CRAY-2 supercomputer (planned for delivery later this year; see article on page 9). The network will also contain a high-performance frame buffer, capable of animating raster images from CRAY memory at effective transfer rates that are expected to exceed 80 MBytes/sec.

Distributed computing, supported by high-performance networking, is another major theme of RIVERS software development. According to Dr. Haber, "The ability to move massive data sets between hosts in an interactive timeframe will lead to a fundamental restructuring of software architectures in scientific and engineering computing. We expect to see simulations distributed across the growing number of machine architectures available on our network, and across the multitiered computing environment—from workstations to supercomputers. The potential for interactive visualization across the network will lead to tighter integration of simulation and visualization software systems." The RIVERS group plans to develop prototype applications to demonstrate run-time monitoring and interactive steering of supercomputer simulations.

Cooperation with computer vendors is a crucial aspect of the RIVERS project. Companies such as Alliant Computer Systems, Apple Computer, Raster Technologies, Silicon Graphics, Sun Microsystems, and Ultra Network Technologies have provided support in the form of discounts, donated equipment, joint development projects, and funding for RIVERS personnel.

Although research and development is the primary mission of the RIVERS group, there are a number of ways that the group's activities will benefit the NCSA user community. Various mechanisms are being established for eventual "productization" of successful RIVERS software projects. The ImageTool software project is one example of how this can occur. ImageTool began as a research project between RIVERS members Mike Norman and Carol Song on a Sun Workstation and was later ported to the Macintosh II by NCSA's Software Development Group with support from Apple (see ***access***, Vol. 2, No. 2). Both the Sun and Macintosh versions of the software are now available (see article on page 17) and supported by NCSA. Dr. Norman and Ms. Song are planning a successor to ImageTool to take advantage of the new high-performance RIVERS hardware systems.

In some cases, agreements between vendors and the RIVERS group include discount programs for the larger NCSA community. For example, all NCSA users can receive a 20 percent discount on purchases of Raster Technologies GX4000 computer graphics board sets for Sun Workstations during 1988. RIVERS is sponsoring a seminar series on Advanced Scientific Computing Environments in cooperation with other NCSA groups. Speakers for the series include Alan Norton (IBM), Roy Hall (Wavefront Technologies), Gordon Bancroft (NASA/Ames), Andries van Dam (Brown University/Stellar), Bruce Borden (Ardent), and Lloyd Treinish (NASA/Goddard).

The RIVERS project is part of a broader effort within NCSA to improve the working environment for supercomputing and computational science. According to Dr. Haber, the most important aspect of the project is that "it will provide NCSA scientists and the vendors a chance to look into the future. We hope to learn about and experiment with the environment that will serve supercomputing users in the 1990s. Given the explosive growth of hardware capabilities, we need prototyping projects such as RIVERS to learn about the software systems needed to harness the computational power that we know is coming."

This three-dimensional view of the updraft in a severe thunderstorm was produced as part of a RIVERS project by Robert Wilhelmson, Crystal Shaw, and Ray Idaszak of NCSA and Joseph Klemp of NCAR. The horizontal horseshoe pattern at low levels indicates that the storm is a potential tornado. *Photo by SMS*

Mathematical Programming Opens New Routes

"At some point early on, I found myself interested in the abstract complexity of urban traffic systems," says David Boyce, UIUC Professor of Transportation and Regional Science in the College of Engineering. This attraction to the mathematical representation of networks is shared by others in the international field of transportation science. Their models of traffic networks are becoming increasingly realistic, thanks in part to the computational powers and memory capabilities of computers such as the CRAY X-MP computer system and to the application of mathematical techniques such as nonlinear programming, a method for solving constrained optimization problems. The rigorous, mathematical approach taken by Dr. Boyce and his colleagues is leading to new methods for modeling dynamic, complex systems—a benefit of interdisciplinary importance.

David Boyce points to a map of the Chicago mass transit systems. *Photo by SMS*

Early Transportation Planning Studies

Urban transportation planning studies in this country began in the Chicago area in 1955 with the Chicago Area Transportation Study (CATS). This was a response to post-war traffic congestion and pressures brought about by large-scale suburban development. From the earliest days of the specialty, transportation planners have attempted to develop models of highway and mass transit systems that accurately describe existing conditions and that can be used to predict the effects of changes such as the addition or deletion of transit lines or roads.

It quickly became apparent that the problems were much bigger than the computers of the day could handle. "They really needed the CRAY supercomputer back in the early '60s," Dr. Boyce notes. For the first 15 years, public agencies in charge of transportation planning worked largely without the benefit of rigorous methods or algorithms. Then about 1970, university graduate students began working on the fundamental modeling problems of the field. Gradually, many of the technical questions stemming from the early studies have been resolved.

Predicting Travel Patterns

In 1980 a collaborative project, funded by the National Science Foundation (NSF) and the Urban Mass Transportation Administration, was begun by David Boyce at the University of Illinois, working with a group of civil engineering graduate students, and Ronald Eash of CATS. The first stage of the project was to develop a model to predict commuters' decisions regarding their best choices of route or mode of transport (car, bus, or train). Later the model was extended to predict people's choices of home or work location.

Building on the work of earlier investigators, the project team developed a model that divides the Chicago region into 300 geographical *zones* and 2500 segments of road called *links.* The Chicago model is now being refined and applied by Swedish graduate student Karin Lennarstrand. She also is working with a similar model based on data from the Stockholm transportation system. Dr. Boyce next hopes to implement the Chicago model using a much larger set of data from CATS with 1800 zones and 30,000 links. This refined model will be more suitable for studies of arterial streets and highways.

Using the CRAY System on the Model

The Chicago model was begun using the State of Illinois computer, an IBM mainframe. In 1986, with a grant from the NSF, Dr. Boyce and former Taiwanese graduate student Chi-Kang Lee moved the research work to the CRAY X-MP computer system. One important advantage of the CRAY system was that the researchers could solve the model in main memory, which allowed them to simplify the code. Another advantage was that for the first time they had sufficient computer time for in-depth study of the properties and performance of the algorithm that solves the model.

Plans for Transportation Modeling

One of the next steps will be to extend the model to consider conflicting traffic flows at intersections, which are largely ignored by current models. Claudio Meneguzzer, a graduate student from Italy, is working on the intersection modeling. Another graduate student, Huey-Kuo Chen from Taiwan, is adapting the code for parallel processing on the Alliant minisupercomputer. In a related thesis research effort, Omar Ben-Ayed, a graduate student from Tunisia, is solving the complex mathematics necessary to identify optimal additions to network capacity.

The goals of transportation modeling for planning purposes almost seem modest when compared to future research plans for electronic route monitoring and guidance systems. These systems will make it possible for commuters to determine their most efficient departure times or routes, using information delivered to them at home or en route. To achieve this goal, the network models will need to be solved repeatedly during the commuting period using current information about traffic conditions. Prototype vehicle guidance systems are being tested in Tokyo, West Berlin, and London.

Adapting Social Science Software

Although transportation planning is his field, Dr. Boyce's research interests extend well beyond the questions of how we get to work or where we live. As chair of the NCSA Social Science Users Committee, Dr. Boyce has organized study groups on adapting optimization software and statistical packages for use on the CRAY system. One optimization package from the University of Arizona that recently became available to NCSA users is XMP. An optimization code developed at Stanford University, named MINOS, is still in the testing stage. Some statistical packages also have been identified by the Social Science Users study group for adaptation, and steps have been taken to acquire them.

Operations Research Advances

Besides developing tools that will enable policy makers to improve urban living conditions, Dr. Boyce and his colleagues are contributing to the interdisciplinary field of operations research. Their studies of the principles that underlie the functioning of complex systems have practical applications in many fields, including communications, economics, health care delivery, and manufacturing.

Advanced computer technology and emerging mathematical methods have enormous potential for contributing to the understanding of complex systems and for evaluating alternative policies for improving their performance. According to Dr. Boyce, the large-scale computing facilities provided by NCSA are making it possible to break through the barriers that have constrained social science modeling for the last decade. "Now," says Dr. Boyce, "the major problem is to make the social science researchers aware of this huge resource that is available to them."

— Kathleen Robinson

Computational Chemist Joins NCSA

Harrell Sellers, Ph.D., joined the NCSA Applications Software Group in late May. His primary responsibilities include working with David Heisterberg and Sam Milosevich to develop a computational chemistry environment at NCSA; helping users get their chemistry-related research under way; maintaining a computational chemistry program library; and continuing his own research projects.

Dr. Sellers is particularly looking forward to heading the effort to establish a strong research environment in computational chemistry, to working with the NCSA industrial partners who are doing molecular dynamics and molecular design, and to continuing his calculations in heterogeneous catalysis.

Other research areas delved into by Dr. Sellers have included theoretical structural chemistry, vibrational quantum chemistry, electron structure theory, metal cluster chemistry, and non-Born Oppenheimer effects. His calculations of the adiabatic correction to molecular potential surfaces were the first of their kind.

Dr. Sellers has worked with a number of eminent researchers in quantum chemistry. Most recently Dr. Sellers was a PACER Research Associate at the Minnesota Supercomputer Institute, where he collaborated with Jan Almlof. Before that he had been on the faculty of Louisiana Tech University, where he was honored with the the university's Outstanding Research Award. Dr. Sellers held a postdoctoral position at the University of Texas at Austin in the research group headed by Jim Boggs and Peter Pulay. His Ph.D. advisors at the University of Arkansas were Neil Ostlund and Lothar Schafer.

"I'm pleased to be at NCSA," said Dr. Sellers. "Right now I'm just getting settled and trying to define and outline the things we want to do here in computational chemistry."

— Stephanie Drake

9600 BPS Service Now at (217) 244-6733

As announced earlier in *access* (Vol. 2, No. 2), NCSA was forced to terminate all 800 numbers as of February 15 due to a budget cut from the National Science Foundation (NSF). NCSA had provided 9600 bps dialin via the toll-free numbers. The 9600 bps service has been restored, but is no longer toll-free. The new number for 9600 bps service is (217) 244-6733.

Computer Program Helps Oil Producers

A new computer technology to aid American oil companies in their revived surge of exploration is being actively transferred to industry by UIUC researchers. The program was developed by Craig Bethke, professor of geology and director of the university's Laboratory for Supercomputing in Hydrogeology, using NCSA's CRAY X-MP/48 system.

The technology, a computer program called Gt, can help companies recover more oil than previously thought available from a reservoir, its developers say. Before production, it examines the chemical reactions likely to occur in a well when it is pumped, aiding in decisions about the best way to bring up the oil.

For example, solid material can form as a result of chemical reactions during pumping, plugging the well and leaving oil behind. If company officials know in advance that this will happen, they can plan a different recovery method and get more oil.

"Below the Earth's surface we can have many thousands of reactions going on at once and it's hard to decide which ones are dominant and which ones are not," Dr. Bethke said. Given data about a particular underground area, the model helps sort it out.

"It's very hard to guess what's going to happen down in a reservoir when you're standing on the surface," Dr. Bethke explained. "Our program offers the ability to look at the reaction between the rock and whatever chemical the company is using, to see what dissolves and what precipitates. This inexpensive calculation can be used to give a prediction of what's going to happen before you find it won't work or will pollute or damage something."

The university is actively transferring this technology to the industrial world. On April 19–21 Dr. Bethke and his colleagues offered a short course entitled "Applied Reaction Path Geochemical Modeling." During the course, researchers from oil companies, well-service companies, and government national labs worked "real-world problems on the computer," Dr. Bethke said.

Oil industry executives recently have said they are boosting their search for new sources of oil and gas in anticipation of a significant shrinking of crude oil supplies in the early 1990s.

— William Allen

Center Activities

AT&T Awards Grant to NCSA

AT&T has awarded NCSA a $700,000 grant to conduct research and implementation in the area of switched (dialup) 56 Kbps (thousand bits per second) networking. The project is funded under the AT&T Academic Affiliate Program and was submitted as part of a UIUC competition. Research will be conducted over the next two years under the direction of Charlie Catlett, NCSA's manager of networking and remote access systems, and Professor Roy Campbell of the UIUC Department of Computer Science.

Switched 56 Kbps service is available in a number of major U.S. cities, as well as between cities via the AT&T ACCUNET switched digital service. This service is not widely used today and represents the beginning of the Integrated Services Digital Network (ISDN), which will provide dialup 64 Kbps and 1.544 Mbps service to every telephone jack, a system that should become a major force by the early 1990s. The project is meant to be a feasibility study of a prototypical ISDN network.

One of the major things we plan to do in the next several months is to improve the lot of NCSA's dialup users. Currently, NCSA offers 1200 bps, 2400 bps, and 9600 bps dialup to center facilities. The NCSA Telnet for the IBM PC software package will be enhanced to accommodate switched 56 Kbps connections so that a remote user with NCSA Telnet will be able to access the center via AT&T ACCUNET at 56 Kbps.

Project researchers will deploy a set of 56 Kbps dialup ports at NCSA that, once software is available, will enable beta site users (chosen by project researchers) to dial in at 56 Kbps via digital modems. Not only will the speed increase, but the software remote users will run will be identical to what is used by local users (TCP/IP's Telnet and FTP utilities) today. This will give remote users a level of performance which, for interactive use, is comparable to the current local network. For file transfer, this service should yield approximately 40 Kbps (today's alternative is Kermit at .8 Kbps to 2 Kbps with a 2400 baud modem).

This is the start of what NCSA expects to be a growing relationship with AT&T. The project has also generated a high level of interest from other companies, and NCSA expects to see similar efforts in this area with such systems as the Apple Macintosh and Sun Workstation.

Also funded under the AT&T Academic Affiliate Program is a project being conducted by the Electronic Visualization Laboratory (EVL) at the University of Illinois at Chicago (UIC). This project is under the direction of Dr. Tom Defanti. The goal of the EVL project is to integrate graphics software tools with AT&T PCs to create interactive scientific animation workstations for remote use. The remote graphics workstation project will rely heavily on the NCSA Telnet software.

— Charlie Catlett

Second Supercomputer Coming to NCSA

NCSA will acquire a second CRAY supercomputer—a CRAY-2/S4-128 system—in an agreement with Cray Research Inc. The University of Illinois Board of Trustees and the National Science Foundation have approved the agreement.

The CRAY-2 computer system is scheduled to be installed in October next to NCSA's current CRAY X-MP/48 system in the Astronomy Building on the UIUC campus, university officials said.

"The acquisition of a CRAY-2 computer at this time is crucial to fulfilling the mission of the National Center for Supercomputing Applications and honors its pledge to provide the most advanced computing resources available to the nation's research community," said Morton W. Weir, chancellor of the UIUC campus.

The CRAY-2 system will enhance the computational power of NCSA and allow researchers to pursue investigations not now possible on the CRAY X-MP system. These investigations require the large memory and other capabilities of the CRAY-2 computer.

An arrangement between NCSA and Cray Research has provided staff and some users with a period of early access to a CRAY-2 system at the company's facility in Mendota Heights, Minnesota, via a high-speed land link. This access enables early familiarization and training with the CRAY-2 architecture and with UNICOS before the NCSA machine is delivered.

The addition of the CRAY-2 supercomputer this fall will provide the computing capacity necessary to satisfy the growing demand for cycles from academic researchers and will allow NCSA to add new corporate partners to its Industrial Program. Current partners are Amoco Corporation, Eastman Kodak Inc., Eli Lilly and Company, and Motorola Inc.

— William Allen

A CRAY-2 computer system. *Photo provided by Cray Research Inc.*

Selected Upcoming Meetings

Science and Engineering on CRAY Supercomputers, Fourth International Symposium, October 12–14, 1988, Minneapolis.
For more information, contact symposium chairman John E. Aldag, Cray Research Inc., 1333 Northland Drive, Mendota Heights, MN 55120-1095, (612) 681-3646.

Workshop on Practical Iterative Methods for Large-Scale Computations, October 23–25, 1988, University of Minnesota, Minneapolis.
For more information, contact workshop administrator, Angie Vail, Minnesota Supercomputer Institute, 1200 Washington Avenue South, Minneapolis, MN 55415, (612) 624-1356.

Supercomputing '88. November 14–18, 1988. Orlando, Florida.
For more information, contact general chairman George Michael, L-306, Lawrence Livermore National Laboratory, P.O. Box 808, Livermore, CA 94550, (415) 422-4239, `gam@lll-crg.arpa`.

Sun Microsystems at NCSA

The Sun Users Group at UIUC has had numerous activities in the past few months, and the presence of Sun systems on the campus and in NCSA is growing rapidly. NCSA now has over 60 Sun Workstations in-house, with the new models 3/60 and 4/260 the most popular. Sun and third-party software for these machines recently has become a topic of considerable interest to NCSA's scientists, consultants, and software development group. Of particular interest have been Sun/CRAY links via tools like NCSA Telnet for the Sun Workstation (Teltool; see articles on page 17 and in this issue of ***data link***) and MicroEMACS (see ***access***, Vol. 1, No. 5). With the release of the NeWS windowing system from Sun Microsystems Inc., there is much interest in developing special graphics tools based on the PostScript language on which NeWS is based.

Customized Support Advocated

On February 11, a Sun Users Group meeting was held at NCSA. Several speakers from Sun Microsystems spoke to about 60 attendees from NCSA and UIUC. The Sun visitors were Diane Cast, university service coordinator from the headquarters office in California; Rich Holada, Marty Polito, and Mike Farley, technical experts or sales representatives from the Chicago office; and Dave Crockett, hardware support representative from Champaign.

Diane Cast, who helps university customers tailor their hardware and software support needs to their systems and budgets, presented several new support programs. One plan, a cooperative self-maintenance system, enables a university employee to train for in-house hardware maintenance, then use a local storehouse of parts to repair systems at a greatly reduced cost. Ms. Cast expressed Sun Microsystems' desire to be as flexible as possible in mixing and matching service features to fit the needs of the customer.

Windowing Enhancements

Rich Holada presented current and future features to expect in Sun windowing system software. The primary windowing product (one that will be included in all future versions of the UNIX operating system from AT&T) is the X.11/NeWS windowing platform. NeWS stands for Network extensible Windowing System and is based on the PostScript page description language familiar to users of the Apple LaserWriter. The NeWS system is based on a client/server model in which your local workstation runs the NeWS server and client machines feed data to the server. The server controls the local windowing structure. Thus, a user on a Sun-3/60, could have one window running color graphics coming from the CRAY X-MP system, another window running input from an Alliant computer, and yet another window from a Sun-4/260 acting as a high-speed Sun compute client. Programs running on the local Sun can also be shown in other windows, of course. The data transfer needed can be much smaller because a short PostScript program can handle considerable graphic information. Versions of NeWS are available for other systems, such as the Macintosh and 80386-based PC systems.

Because X.11 has been selected by some vendors as a standard, Sun Microsystems is also supporting X.11 merged with the NeWS system. A new version of the standard Sun windowing environment, SunView 2.0, is being designed on top of the X.11/NeWS platform. You will be able to run X.11, NeWS, and SunView windows simultaneously on the same Sun screen. The full system will become available in the fall of 1988 when the 4.1 version of the SunOS UNIX software is released. NeWS version 1.1 is now available at a nominal price to university users on the Sun-3 and Sun-4 systems. With the recent agreement between Sun Microsystems and AT&T on future developments in the UNIX software, the X.11/NeWS combination will become a standard part of the UNIX that is licensed to all vendors.

Help Session and New Product Discussion

During the help session, Mike Farley and the other Sun representatives fielded technical questions regarding Sun use. The meeting concluded with Mike Farley and Marty Polito discussing the future of Sun UNIX software and demonstrating the new Sun-4/110 desktop system that is based upon the Sun SPARC reduced instruction set computer (RISC) chip. This system offers a large variety of monitors and disk options and is ideal either as a server for a small network of Sun-3s or as a high-performance single user machine.

Future Trends for Sun at NCSA

On February 25, Curt Wozniak, Phil Heller, and Sina Tamaddon visited NCSA to discuss a potential growing relationship between Sun Microsystems and NCSA. Sun has recently announced an alliance with Cray Research Inc. NCSA is in an ideal position to participate in the development of high performance workstation/supercomputer interfaces.

Mr. Wozniak is a vice president for the educational market at Sun, and Mr. Heller and Mr. Tamaddon are well known Sun university representatives who have played a major role in making Sun successful in the scientific and educational markets. Mr. Tamaddon is a "Sun guru" whose expertise is always in high demand. He is also a physical chemist.

Future meetings for the Sun User Group will include a roundtable discussion of software for the Sun Workstation and detailed technical talks on UNIX, NeWS, and the LISP programming environment. Also expected are visits and talks by top software and hardware developers at Sun as well as demonstrations of more new products. A list of the software currently running on NCSA Suns (more than 100 programs) is being compiled so that NCSA's local and remote Sun users can have some idea of the software now available.

— Steve Christensen

NCSA Director Smarr Testifies Before Congress

NCSA and the other NSF Phase II supercomputer centers have strengthened the national scientific infrastructure and increased America's international competitiveness, but continued success requires a "stable, predictable, and adequate" base of federal funds, Larry L. Smarr, NCSA director, testified at a congressional hearing on March 24.

"We have shown that Computational Science and Engineering is a powerful new force for the future of our country," Dr. Smarr testified before the U.S. House Subcommittee on Science, Research, and Technology. "We have many good examples of how pioneering researchers can use their new-found access to supercomputers and advanced visualization techniques to open new fields. We have planted the seeds of hope in an entire new generation of graduate students and faculty with education and training programs. And we have been successful in persuading a number of major corporations to join in enlarging the program.

"If we can keep the commitments made by each partner to our shared vision, then we will witness a continual increase in the academic and industrial application of our country's most advanced technologies."

Critical Need for Increased Support

Dr. Smarr said Congress, the NSF, and the supercomputer centers should be proud of "an incredible achievement in a very short time," but that the need for reliable federal support is "particularly critical at this point in the history of the program."

At the hearing, which was held to examine the proposed NSF budget for fiscal year 1989, Clifford E. Rhoades Jr., deputy division leader for computational physics at Lawrence Livermore National Laboratory and head of an NSF study of the five centers, testified that "the national supercomputer centers are in crisis."

Dr. Rhoades said recent federal budget cuts have hurt development of the national supercomputing network, lowered staff morale at the centers, and begun to "turn off" students and researchers to the promise of computational science—trends that will have "profound effects on science, technology, and industry in America."

Recommendations for Funding Agencies

Dr. Smarr called on the federal government to renew its commitment to double the NSF research budget over the next five years, to guarantee an increase for basic research, and to provide the NSF supercomputer centers with "predictable and stable funding with a rolling five-year horizon." He urged Congress and the NSF to maintain the centers at "the leading edge of computing technology" and to add new supercomputing capacity as soon as possible to saturated centers.

He supported Dr. Rhoades' recommendation that the cooperative agreements between the NSF and the centers have automatic federal matching funds for new funds raised by the centers outside those anticipated by the cooperative agreements.

Facilities Also Require Upgrades

With regard to national network access, Dr. Smarr called for accelerated upgrading of the NSFnet, encouragement of universities to install effective local area networks to link the user's research office or lab to the campus gateway and NSFnet, and setting a national goal of creating a billion byte-per-second national "information superhighway" of optical fibers within the next decade.

— William Allen

Training Sessions Scheduled for New Computer Users

NCSA offers intensive two-day training sessions for users—particularly new users—of NCSA's CRAY computer system. These user training sessions and laboratory exercises provide information and practice necessary for getting started with the various NCSA systems. Topics include the CTSS operating system, the DDT debugger, job control, software packages, and code optimization and vectorization. Enrollment is limited.

New user training sessions are scheduled for:

June 27, 28
July 25, 26
August 29, 30
October 3, 4
November 7, 8
December 5, 6

To register for a training session, phone Tammie Hildreth at (217) 244-8306. For more information about the training program, contact Alan Craig at (217) 244-1988 or via the BITNET address `training@ncsavmsa`. To see the latest training schedule, enter `help training` on the VAX or CRAY computer.

If you would like to extend your visit at NCSA beyond the training program dates, phone Patricia Wenzel at (217) 244-0072 regarding the NCSA Visitors Program.

Peer Review Board Meeting March 8

The joint NCSA/Pittsburgh Supercomputing Center (PSC) Peer Review Board (PRB) meeting was held on March 8 in Washington, DC at the NSF. Several NSF program directors attended the meeting to gain a better understanding of what is required of their grantees who apply for supercomputing time.

Junko Shigemitsu of Ohio State University and Bert Green of Johns Hopkins University resigned from the board. PSC director Ralph Roskies is working with NCSA to find replacements in physics and the social sciences. Barry Kline of the Naval Research Laboratory and Ray Chin of the NSF each attended for the first time.

NCSA indicated to the board that its resources are overallocated. NCSA is addressing this by making changes to its allocation policy (see ***access*** Vol. 2, No. 2). The backlog of projects waiting to be put on the CRAY X-MP computer system amounts to approximately 5000 service units (SUs), and new projects are being added only as old projects expire. Also, NCSA has instituted a new policy for extending the expiration date of projects: only 25 percent of unused SUs are being extended for a maximum period of six months.

SUs allocated by the PRB were as follows:

PSC	3345 of 7425 requested (45%)
NCSA	385 of 1490 requested (25%)

In the past, NSF allocated a portion of the time available on the supercomputers at the five supercomputing centers, and the centers allocated the remainder. In the future, all the time will be allocated by the local boards. A researcher can still apply directly to NSF for supercomputing time, but NSF will forward the application to the local board with an allocation recommendation. The local board will then make a full or partial allocation based on available SUs.

As the supercomputers have become more heavily loaded, the members of the joint NCSA/PSC board have become more stringent in their reviews of proposals. In addition to evaluating the content of proposals, the board members appreciate those proposals that:

- stay within the guidelines for length.
- are clearly written for a nontechnical audience.
- contain all the necessary supporting materials.
- contain an up-to-date curriculum vita.

For supplemental requests, the PRB members like to have available a preprint or reprint of any published articles pertaining to completed research.

The PRB meets quarterly in June, September, December, and March. To allow adequate time for the review process, applications should be sent to NCSA by the first of the month prior to the meeting date.

— Patricia Wenzel

Visitors at NCSA

Ken Bishop. Sept. 27, 1987–Aug. 1, 1988 from University of Kansas. Area of research: petroleum engineering.

Charles Evans. May 3–14 from California Institute of Technology. Area of research: astrophysics.

Sam Finn. May 2–14 from Cornell University. Area of research: astrophysics.

Phil Hardee. May 23–26 from University of Alabama at Tuscaloosa. Area of research: astrophysics.

John Hawley. May 8–19 from University of Virginia. Area of research: astrophyics.

Nick Kazarinoff. May 2–18 from SUNY–Buffalo. Area of research: mathematics.

Chris Kochanek. May 8–18 from California Institute of Technology. Area of research: astrophysics.

Mordecai Maclow. May 13–27 from University of Colorado. Area of research: astrophysics.

Grant Mathews. May 2–14 from Lawrence Livermore National Laboratory. Area of research: physics.

Richard Matzner. May 11–14 from University of Texas. Area of research: astrophysics.

Anthony Mezzacappa. May 5–14 from University of Texas. Area of research: astrophysics.

Michael Minkoff. May 4–6 from Argonne National Laboratory. Area of research: mathematics and computer science.

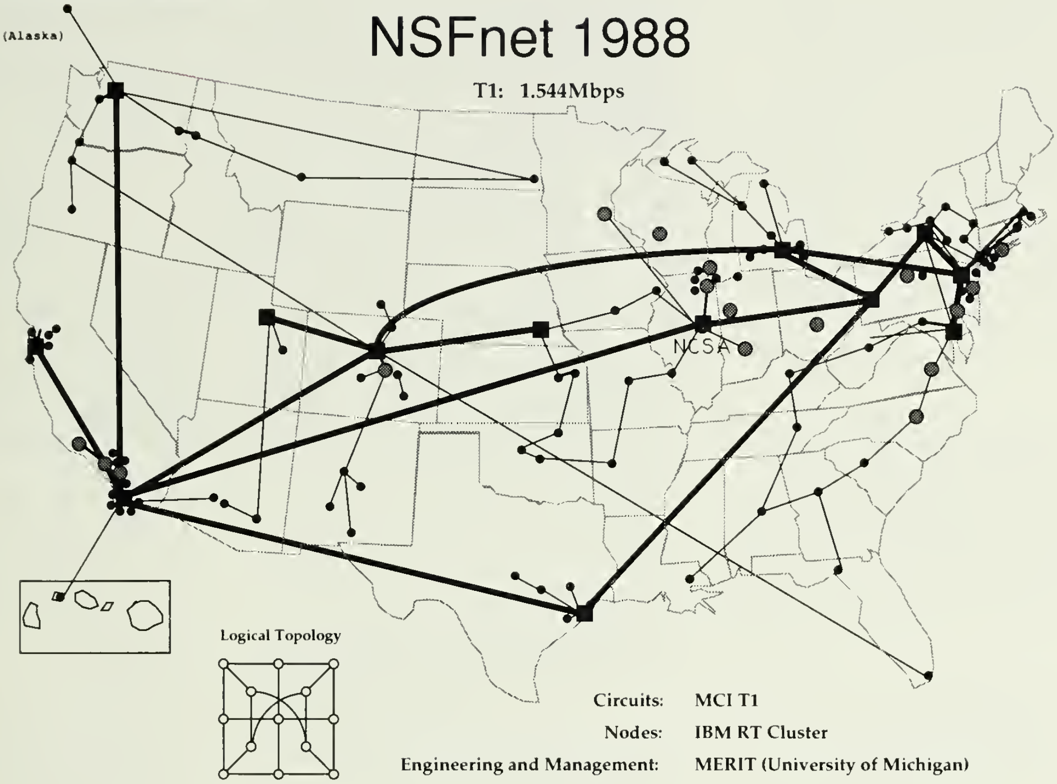
Joel Rauber. May 23–August 1 from South Dakota State University. Area of research: astronomy.

Klaus Schulten. April 1–30 from University of Illinois. Area of research: physics.

M. A.Venkataramanan. May 30–June 10 from Indiana University. Area of research: management science.

Nathaniel Whitaker. April 24–28 from University of Massachusetts. Area of research: mathematics.

Networking



NSFnet 1988

T1: 1.544Mbps

Circuits: MCI T1
Nodes: IBM RT Cluster
Engineering and Management: MERIT (University of Michigan)

New NSFnet Backbone

The NSF has funded a proposal cosponsored by Merit Inc., IBM, and MCI for a new NSFnet backbone. The new backbone will consist of the six existing backbone nodes, as well as seven new sites (see map). After the backbone becomes operational, NSFnet users can expect more reliable connections as well as increased performance.

With the addition of the seven new backbone nodes, each of the NSF-funded regional networks will have a primary backbone node located on its network. With the current backbone, multiple regional networks share backbone nodes. For example, currently BARRNET, SDSCnet, and NorthwestNet share the SDSC backbone node. With the new backbone, each of these three networks will have its own backbone node. MIDnet, the regional network connected to the NCSA backbone node, will now have a primary backbone node located at the University of Nebraska at Lincoln campus and will maintain the connection to NCSA as its secondary node.

The backbone itself will be composed of T1 data links, provided by MCI, that send data at a speed of 1.544 Mbps (million bits per second). This is 24 times faster than the existing links that run at 56 Kbps (thousand bits per second). IBM will supply equipment for each of the backbone nodes. This equipment will include IBM PC/RTs and PS/2s linked together by an IBM Token Ring network. The Network Operations Center (NOC) will be centered in Ann Arbor, Michigan and will be run by Merit Inc., which has successfully managed the Merit Computer Network in Michigan for nearly 15 years.

Implementation of the new backbone is divided into three phases. Phase one of the proposal includes a cutover to the T1 lines, the IBM equipment, and the Merit network management from the existing backbone. The phase one cutover date is July 1, 1988. The second phase, scheduled for early 1989, will give network operations the ability to dynamically reconfigure the T1 connections between given sites. This means that if the connection between two backbone nodes is highly congested, causing poor service, additional bandwidth can be allocated to that connection. This decreases traffic congestion and session delays. This dynamic reconfigurability is a service provided by MCI. The final phase of the proposal involves an upgrade from T1 data service to T3 data service,which runs at 45 Mbps. This phase is planned for operation sometime in 1990.

In the past several months, NCSA has received a number of reports from users regarding problems with the current NSFnet. These problems are due largely to an increasing number of regional network connections that increase the load on the backbone. With the upgrade in capacity and the doubling of the number of backbone nodes, users should expect to see a measurable improvement in both reliability and performance.

— Steve Crumb

Improved Connections to ARPANET

Through the efforts of the Computing Services Office of UIUC, a new ARPANET connection has been established that improves connections to NCSA from organizations on the ARPANET. The new connection, which is a 56 Kbps (thousand bits per second) line to the University of Wisconsin at Madison node, has been in service since early March.

Before this connection was established, ARPANET traffic had to be transmitted across the NSFnet backbone through the Pittsburgh node. This added to the load of the NSFnet backbone as well as the Pittsburgh NSFnet/ARPANET gateway. Now, ARPANET traffic to NCSA can be routed directly through the independent UIUC/NCSA connection.

This new connection not only improves NCSA's connectivity to the ARPANET, but also reduces the load on the NSFnet backbone by providing another location for moving packets from one network to the other. This is good news for connections to NCSA over the NSFnet because draining the ARPANET traffic eases NSFnet congestion around the UIUC/NCSA node.

— **Steve Crumb**

Academic Affiliates

An Innovative Supercomputing Training Program

With the support of the National Center for Supercomputing Applications, other supercomputing centers, and the computing industry (Cray Research Inc. and IBM), the University of Illinois at Chicago (UIC) is offering a new kind of educational opportunity to people in computing-intensive research areas who need to understand the role and use of modern computational tools in their research.

This training program is an alternative to the short courses offered by supercomputing centers to instruct new users how to use a specific supercomputer and to the universities' academic courses to teach scientists and engineers about some aspects of supercomputing.

The UIC Graduate Student Workshop Program on Scientific Supercomputing is being developed as a model program for the integration of advanced architecture computing techniques into the research training of scientists and engineers. This program attempts to expand the knowledge base of advanced computing into the "practicing" scientific and engineering fields. The training program arises from a strongly felt need among the UIC faculty. It uses as the basis for supercomputing the same network connection to the NSF-sponsored national centers used by researchers to access supercomputers.

Special Features of the Program

The features that make this program unique and that contribute to its promise are:

- An 11-week immersion program, free from distractions of other coursework or teaching responsibilities.
- Seminars on concepts and issues by visiting lecturers—users, vendors, computer scientists, mathematicians, scientists, and engineers from academic departments, computing and research centers, and the computing industry—each an expert in his or her own field.
- Pursuit of participants' research objectives by implementing their application programs on a variety of supercomputers to explore the nature of supercomputer architectures and their effects on the applications.
- Four to six graduate or postdoctoral students from different scientific and engineering disciplines, including computer science. Students develop a sense of team work, encouraged by student presentations, debugging sessions, and the exchange of scientific viewpoints.
- Library of books, journals, supercomputer manuals, articles on computer optimization, mathematical libraries, videotapes, and online bibliography. Participants study the literature and discuss different published approaches to scientific computing problems.
- Guided tours of how to read and debug programs, including code written by others, a very important part of every scientist's professional life.
- Site visits to supercomputing centers for in-depth work on programs with resident experts.

Visits to NCSA

Students from the fall and winter quarters visited NCSA for one day in January, and students from the spring quarter were at NCSA for two days in May. They worked with their own application programs on the CRAY X-MP/48 computer system with the assistance of NCSA consultants, and they had the special opportunity to use Sun Workstations as front-ends to the CRAY supercomputer.

Participants were able to see their data in a new way, using a variety of graphics analysis tools on the Sun. Their complex data sets came to life with the use of 3D color graphics, which made it possible to see great detail.

The UIC supercomputing class visiting NCSA's CRAY X-MP in January. Left to right: James Choi, Li Zhou, Nazeer Shareef, Anil Manhapra, Vanessa Jub, Nora Sabelli, Ann Solem, Matt Hettinger. *Photo by SMS*

Program Sponsorship and Support

The program is jointly sponsored by the Academic Computer Center and by faculty from the Department of Mathematics, Statistics, and Computer Science and the Department of Electrical Engineering and Computer Science, both at UIC, with funds from the Graduate College and the Academic Computer Center.

NCSA has sent graphics and visualization experts each quarter. Similarly, two computer vendors (IBM and Cray Research Inc.) have sent technical speakers from Los Alamos NM; Minneapolis MN; and Kingston, NY. In addition, IBM has provided the microcomputers used as workstations by program students; has paid for a vectorization fellow to work in close association with the program, partly as a teaching assistant and partly to learn our approach; and has paid for a visit by the student participants to IBM's Kingston Laboratory for four days of in-depth analysis of parallelization.

What Instructors and Students Learned During the Initial Program Phase

The most important conclusions were that:

- The "immersion workshop" approach was extremely successful and led to a qualitative change in participants' understanding of the process of computing and its relation to their scientific aims.
- Direct exposure to vendors in a technical context was an important part of the learning experience.
- Repetition of presentations by the students as their work progressed was very useful to the students themselves.
- Close participation of students' research advisors was an important resource in increasing students' understanding of other computationally intensive research areas.
- Site visits were important to the sense of growth, research of computing trends, and camaraderie among participants.
- Every participant learned basic computing and debugging techniques during the program that would have been useful in software development before the program; there is no mechanism in place for nonprogrammers to learn what can be termed "good programming habits," because these are still passed in an apprenticeship context, and professional scientific computer programmers are not common in universities.

The best way to show the success of the program is through its effect on alumni.

One participant, funded by his advisor, was able to increase by a factor of three the speed of the program his group was using. His careful benchmarking demonstrated an error that cropped up after 4000 iterations and opened the way for making his group's results more accurate.

Another participant was asked by his department head to make a presentation to the whole department on his timing benchmarks on finite element program optimization. Now working as a teaching assistant in an advanced CAD/CAM course, he reports that the debugging techniques and ability to read other people's programs developed during the workshop are as useful in his role as the factual information he acquired.

Because of their new understanding of fundamental concepts and their newly perceived need for information, two engineering alumni will take computer science classes next fall in numerical algorithms and introduction to computer architecture.

One participant's interaction with an alumnus in a different field helped him devise a new, more efficient algorithm for his program that may prove to reduce execution time significantly.

The Future of the Program

Once firmly established, a program of this nature requires minimum additional funding, running well just on funds for the coordinator's time and graduate student assistantship.

UIC plans to develop the Workshop Program on Scientific Supercomputing as a model program that can be adopted by other affiliates. The group will develop curricula and course materials that can be distributed to other institutions and will be happy to help set up similar programs elsewhere.

— Nora Sabelli and Ann Solem
University of Illinois at Chicago

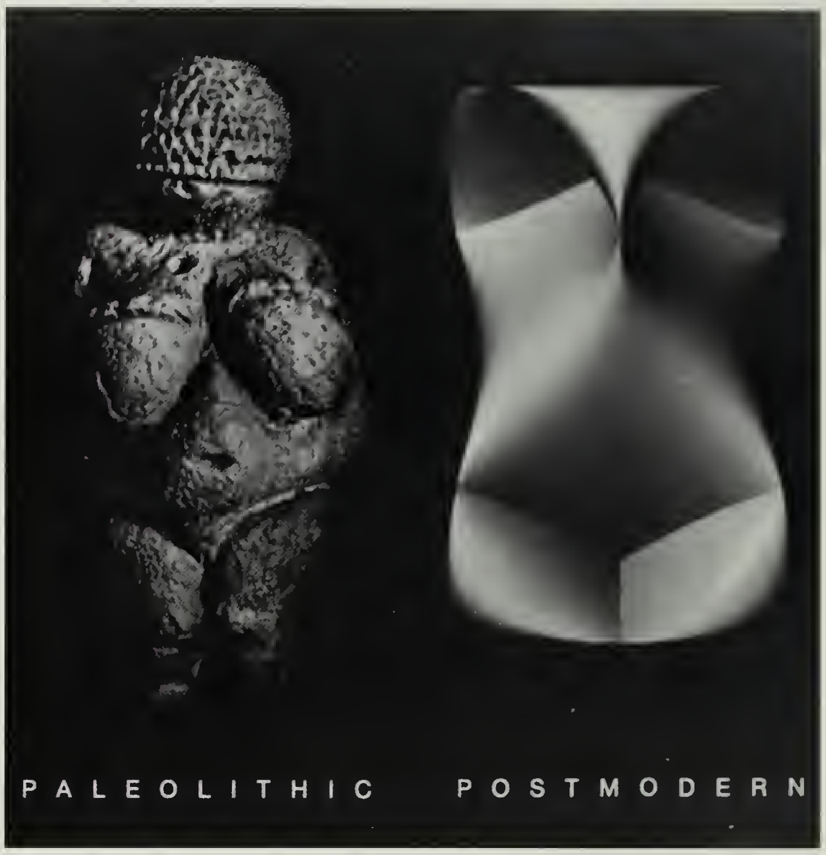
Basic Training for Affiliates

NCSA hosted its third PHASE I training week for the NCSA Academic Affiliates Program on March 5–9. The PHASE I session trains an academic affiliate contact to be an on-site NCSA consultant for researchers at an affiliate campus. During their week at NCSA, affiliate contacts gain exposure to the center and meet many NCSA staff. The training program covers the technical aspects of NCSA from workstations to the CRAY computer system, the organization of the NCSA Academic Affiliates Program, and the rights and responsibilities of an academic affiliate campus.

Donna Cox, Professor of Art and Design at UIUC and visiting faculty at NCSA, addressed the group of 40 affiliates on computer graphics and her concept of "Renaissance Teams: A Convergence of Art and Science." Her presentation covered historical precedence and included descriptions of NCSA projects in which scientists, artists, and computer specialists have collaborated to create scientific visualizations.

Each new affiliate institution received a Macintosh SE, donated by Apple Computer Inc., and NCSA software for the machines to take to its home campus. There are currently over 60 NCSA academic affiliates. For more information about the NCSA Academic Affiliates Program, contact Alan Craig at the BITNET address `13020@ncsavmsa` or at the Internet address `acraig@newton.ncsa.uiuc.edu`

— **Alan Craig**



During her presentation to Phase I affiliates, Donna Cox used these two images of Venus to explain the concept of Renaissance Teams. "Like the supercomputer-generated postmodern Venus, the paleolithic Venus was made with the best technology of its time. It is believed that the belly of the Stone Age Venus was rubbed to bring greater fertility to its tribe. Similarly, the supercomputer Venus is massaged with twentieth-century computational techniques to bring greater understanding to mathematical thought. Unlike the Stone Age Venus, the supercomputer form was created by a team of experts in the quest for knowledge and discovery. Because disciplines have become specialized and diversified, the future belongs to interdisciplinary Renaissance Teams: teamwork between humans and technology, between artists and scientists, between academia and industry." *Photo by SMS*

Advanced Training for Affiliates

During the week of February 15–19, NCSA hosted its first PHASE II training session for the NCSA Academic Affiliates Program. This advanced session is for affiliate consultants who have completed an NCSA PHASE I training session and require knowledge of advanced subjects. The PHASE II session covers additional material, more technical concepts, and updates to material covered in the basic training session.

Thirty-six affiliates returned to NCSA for the additional week of training. Topics on the agenda included graphics, workstation developments, new NCSA software, parallel processing, the Alliant FX/8, job control on the CRAY computer, and an in-depth look at the CRAY X-MP architecture and code optimization.

A highlight of the week was the dinner with invited speaker Robert Haber, professor of civil engineering at UIUC and visiting faculty at NCSA, who spoke to the group about advanced interactive scientific visualization and the RIVERS project. (See page 4 for more information about the RIVERS project.) Dr. Haber emphasized the need for interactive visualization tools and high-performance network systems.

Some of the attendees said that one benefit of the program was the chance to interact with other experienced affiliates to share ideas and exchange information. The feedback from the affiliates is also valuable in helping NCSA to develop and improve. For more information about the NCSA Academic Affiliates Program, contact Alan Craig at the BITNET address `13020@ncsavmsa` or at the Internet address `acraig@newton.ncsa.uiuc.eduCc.edu`

— **Alan Craig**

Software

Symbolic Manipulation Systems at NCSA

A major interest in symbolic manipulation systems (sometimes called *computer math* or *computer algebra systems*) has grown over the past few years. The reason for this is the emergence of very high-speed, large-memory personal workstations such as the Sun Workstation. In the past, many computer algebra systems could run only on mainframes or departmental minicomputers and were therefore not always accessible or usable due to their considerable draw on system resources. This has changed with today's workstations, and much new development is going on.

This article mentions some of the symbolic manipulation systems now available and gives a glimpse of future developments. Numerous systems are now available, but I focus first on systems for Sun Workstations and then discuss systems for CRAY X-MP/48 and Macintosh computers.

The Sun Workstation is now the computer of choice for running and developing symbolic manipulation systems. In particular, the Sun-4—with its high speed, memory of potentially 128 megabytes, and fast local disks—is likely to become the ideal platform for almost any level of work in this area.

Symbolic Math Software Running at NCSA

Here at NCSA the following systems are running on Sun-3s or Sun-4s at various levels of use and support:

- Mathematica (beta test)
- Macsyma
    Symbolics Macsyma version 309.6
    DOE Vaxima version 2.10 (just released)
    DOE Maxima version (Common LISP version)
- SMP version 1.60
- Maple version 4.1
- Reduce version 3.3

Sheep version 2.52 is being ported to the Sun-3, and NCSA is testing versions of a number of unannounced alpha and beta test products for the Sun-3 and Sun-4. NCSA is also in the process of obtaining Cayley.

All of these systems have had recent major upgrades and additions of libraries too numerous to mention here. No system is currently recommended over the others because each has its own strengths and weaknesses. Upgrades in the level and quality of documentation have also been made in every case, so these programs are much easier to use.

In general, the LISP-based systems require more memory both in RAM and disk space. The Symbolics and Vaxima versions of Macsyma are currently based on Franz LISP dialects, while the

Symbolic *continued on page 19*

Now Available—

Contours for the Macintosh version 1.1

Contours for the Macintosh generates contour, 3D, and shaded intensity plots from raster files. Contours has been enhanced and version 1.1 is now available. Contours features now include two alternate methods of selecting contour levels: you can select the number of contour lines to be drawn, or you may specify the individual values at which you would like the lines drawn.

To order software and documentation for Contours, complete the order form in the *NCSA Technical Resources Catalog* or telephone (217) 244-0072. The cost is $11.50 for software and documentation. Ordered separately, software is $10.00 and documentation is $1.50. You may also get Contours from anonymous FTP (see below).

ImageTool for the Sun Workstation version 1.0

ImageTool for the Sun Workstation version 1.0 provides a color raster image display capability; it can generate XY graphs, contour plots, and 3D plots from raster files on a Sun Workstation. Palette modification utilities are also provided. For more information, see the ***data link*** article in this issue.

ImageTool for the Sun Workstation is distributed in two parts. The source code and executables have been added to the anonymous FTP source distribution, and the documentation is sold separately.

To order ImageTool for the Sun Workstation, telephone (217) 244-0072. The cost is $50 for the source cartridge tape and $30 for the source reel tape. The documentation is $2.50. You may also get the software from anonymous FTP (see below).

ImageTool for the Macintosh II version 1.1

ImageTool for the Macintosh version 1.1 is now available from NCSA. This update provides a color raster image display capability; it can generate contour, 3D, and shaded intensity plots from raster files on the Mac II. Palette modification utilities are also provided. Version 1.1 features a friendly user interface and support for Hierarchical Data Format (HDF), NCSA's new graphics file format.

To order the software and documentation for ImageTool for the Macintosh II, complete the order form in the *NCSA Technical Resources Catalog* or telephone (217) 244-0072. The cost is $12.50 for software and documentation. Ordered separately, the software is $10.00 and documentation is $2.50. You may also get this software from anonymous FTP.

To use anonymous FTP, start up FTP and connect to the anonymous FTP (the IP address is `128.174.20.50 decimal`) by entering `ftp.ncsa.uiuc.edu`. Log on as `anonymous` and specify your name for the password. Each directory contains a `readme` file describing the distribution, which should be read first. For more information, call the NCSA consulting office at (217) 244-1144.

—**Tom Redman**

Picture This

According to a familiar saying, a picture is worth a thousand words. At NCSA, Scientific Media Services (SMS) produces valuable "pictures" or visual records. The group outputs visual imagery, documents the center's activities pictorially, and maintains the center's output devices. Its assignments range from producing videotapes of images generated by scientific research to photographing staff members to keeping public printers stocked with paper at NCSA's Interdisciplinary Research Center (IRC).

"Most of our output is video or film," says Dan Brady, SMS administrator. For example, scientists doing research on the CRAY X-MP/48 system have their data converted into images. With an Abekas A62 digital video storage device, SMS uses that data to produce a videotape which shows a step-by-step progression in some research finding. In the editing process, explanatory titles may be added to the video. Consultants assist scientific investigators and act as liaisons between SMS and principal investigators (PIs) to work out the best approaches in the imaging process.

SMS's functions include recording image files from an Alliant FX/80 to video, duplicating animations, copying videotapes, and recording images on either slide or print film. Titles and logos to annotate and credit videotapes and slides are created by SMS. In image digitization, images input through a video camera can be modified with the Lumena paint system and/or transferred to the Alliant FX/80. Principal users of these services are the Scientific Visualization Program, visiting scientists, industrial partners, and staff scientists. For instance, the Scientific Visualization Program staff create three-dimensional visualizations of research data and use SMS facilities to record and sequence the output. Plans are being considered to open SMS's services to remote users in the future.

SMS also documents the science that is being carried out at NCSA by creating and producing video programs. These video programs are often used in presentations promoting the center by the Director's Office and the NCSA Industrial Program. Other video productions serve as training tools for NCSA's academic affiliates, remote users, and research scientists.

The SMS staff. From left to right: Ingrid Kallick, Vincent Jurgens, Cordelia Baron, Steve Blakey, and Dan Brady. *Photo by SMS*

Photographing NCSA people, places, and equipment records the center's growth and history. Most of the photographs in this issue of ***access*** were shot by SMS, for example. Slides to illustrate technical reports are produced as well. SMS also contracts with outside organizations for photo lab services as well as video production work when necessary. In April, SMS coordinated the production of a live, interactive teleconference ("Molecular Design Using Supercomputers" from the San Diego Supercomputer Center) with a video production facility that handled the presentation mechanics via satellite.

As the collection of slides and videotapes produced at NCSA grows, it is becoming a database that requires management. To that end, SMS is indexing and cataloging its collection of videos and slides systematically, like a library. This archiving process will benefit potential users by allowing them to retrieve images and data.

Who Are the SMS staff?

Dan Brady, whose expertise is in video production, describes his central focus as working with communication systems and keeping abreast of future developments in the field so that new technology can be implemented here at NCSA. He also searches out "anything new" developing in graphics.Vincent Jurgens, coordinator of operations, sets daily priorities, supervises the student assistants, and assists in video project development.

Student post-production (editing) operators are: Ingrid Kallick, graduate student in graphic design; Cordelia Baron, undergraduate in film studies; and Steve Blakey, undergraduate in photography. Although they engage in all SMS's activities and "do everything," each student specializes somewhat. For example, Ms. Kallick prepares titles and graphics; Ms. Baron does production and video; and Mr. Blakey, formerly a computer science student, provides programming skills.

What Are Future Media Service Plans?

SMS hopes to enhance its services to scientists by using more sophisticated presentation techniques for video programs, according to Dan Brady, although this is contingent on funding. Besides imaging sequences from research data, further annotation of the images would be provided with upgraded equipment for titling and other graphic effects. Compositing techniques would combine multiple viewports, or windows, into a single frame. To further clarify research, voice-overs and on-camera commentary describing scientists' work would be employed. Video programs that more effectively communicate NCSA's scientific research would significantly enhance the flow of information in today's scientific communications media.

— **Fran Bond**

Symbolic continued from page 17

Maxima version is written in Common LISP. All of these systems come with a multitude of "share" libraries for special-purpose calculations. Symbolics has announced that a Common LISP version of their Macsyma for Sun Workstations will be available in the latter part of 1988. Reduce is written in Portable Standard LISP, while Maple, SMP, and Mathematica are written in the C language.

One of the more active areas of work in symbolic manipulation systems is the creation of user-friendly interfaces so that the input and output of the programs looks like normal equations or graphs. Several such systems built within the NeWS or X-windows are now in beta test at various places, including NCSA.

The programs mentioned here exist on other computer systems. Maple, Reduce, and Mathematica currently run on the Macintosh. Reduce runs on the CRAY X-MP system and Maple has a CRAY-2 version. NCSA expects that most of the systems eventually will be ported to the UNICOS CRAY-2 system.

Supercomputer versions of symbolic manipulation systems are really best used in batch production modes for very large problems, because Sun Workstations and Macintoshes are much better for this kind of highly interactive work. It is hoped that in the future, the combination of highly interactive modes on a workstation with the extremely high-speed, very large memory capabilities of supercomputers will provide extraordinary "symbol crunching" tools to any scientific or engineering user.

NCSA Contacts

Academic Affiliates	217-244-1988 `13020@ncsavmsa` (BITNET) `acraig@ncsaa.ncsa.uiuc.edu` (Internet)
Industrial Program	217-244-0474
Consulting Office	217-244-1144 `consult@ncsavmsa` (BITNET) `consult@ncsaa.ncsa.uiuc.edu` (Internet)
CRAY Operations	217-244-0710
NCSA Receptionist	217-244-0072
New Accounts/Users	217-244-0074 `uadmin@ncsavmsa` (BITNET) `uadmin@ncsaa.ncsa.uiuc.edu` (Internet)
Training Program	217-244-1988 `training@ncsavmsa` (BITNET)
Visitors Program	217-244-0074 `uadmin@ncsavmsa` (BITNET) `uadmin@ncsaa.ncsa.uiuc.edu` (Internet)
VAX Telenet Address	217 35
CRAY IP Address	`ncsad.ncsa.uiuc.edu` (128.174.10.48)
Front-end VAX BITNET Address	*user*`@ncsavmsa`
Front-end VAX IP Address	`ncsaa.ncsa.uiuc.edu` (128.174.5.100) `ncsab.ncsa.uiuc.edu` (128.174.5.101)
NSFnet Problems (NSF Network Service Center)	617-873-3400 `nnsc@nnsc.nsf.net`
ARPANET Problems (SRI-Network Information Center)	800-235-3155 415-859-3695 `nic@sri-nic.arpa`

New Electronic Mailing List of Sun Users

To further the use and development of symbolic math programs, an electronic mailing list has been started to promote the exchange of information on software for Sun Workstations. Correspondence and articles are collected and sent out to the mailing list roughly once per week. Currently there are approximately 100 people on the list representing users in the United States, Canada, Australia, England, and other countries. At the request of the International Sun User Group, I started and maintain the list.

Anyone who would like to be added to the mailing list can send his or her electronic mail address via Internet to:

`Sun-Symbolic-Math-Request@spock.ncsa.uiuc.edu.`

Correspondence and articles can be sent via Internet to:

`Sun-Symbolic-Math@spock.ncsa.uiuc.edu.`

— **Steve Christensen**

data link Preview

Vol. 2 No. 3

Analyzing Application Performance—CRAY X-MP Hardware Performance Monitors
The CTSS operating system has recently been modified so that users can monitor FORTRAN programs through the CRAY X-MP/48 computer's hardware performance monitor counters.

A Fast Linear System Solver
A routine called `lusp` outperforms most system solver routines for a wide range of matrix orders. `lusp` is a highly optimized routine (partially written in Cray Assembly Language) that performs the LU decomposition using the Gaussian elimination.

File Transfer on the Macintosh
This article discusses many of the formats and programs developed to help Macintosh users overcome problems transferring data to and from other computer systems.

IMCOMP—An Image Compression and Conversion Algorithm for the Efficient Transmission, Storage, and Display of Color Images
IMCOMP, a set of image conversion and compression routines, allows users of the CRAY X-MP computer to convert images to 16- or 8-bits per pixel, and then to compress them further to 2- or 3-bits per pixel while maintaining a reasonable full-color representation.

Improving Interactivity on the CRAY X-MP/48 System
This article describes how changes to CTSS provide better interactive response time.

Message of the Day on the CRAY
This article explains the new information printed when you log on to the CRAY computer, including the time of last login and a "message of the day."

NAGHELP—Online Documentation for NAGLIB
Naghelp, the NAG Interactive HELP System for Mark 11 of NAGLIB, is now available on the NCSA CRAY X-MP computer to serve as an online source of information that complements the published FORTRAN library manuals.

NCSA Mass Storage System
This article provides information on the NCSA mass storage system and presents recent usage statistics.

New Color Imaging Program—ImageTool for the Sun Workstation
NCSA introduces ImageTool, a program that allows the scientist to "see" the data created on the CRAY X-MP computer system.

TOEPLITZ Package Available on the CRAY X-MP System
The TOEPLITZ package solves sytems of linear equations with coefficient matrices of Toeplitz or circulant form.

data link is a collection of technical articles for NCSA computer users. If you do not receive ***data link***, but are interested in one of the above articles, call NCSA at 217-244-0072 to get a copy of this issue. If you want to receive ***data link*** on a regular basis, fill out the subscription form below

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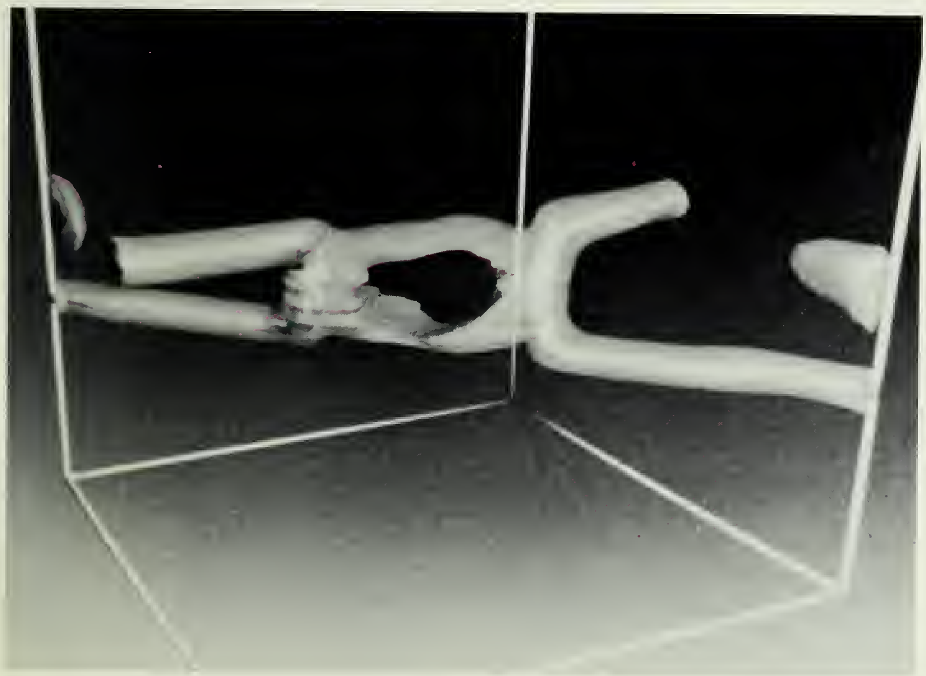
Science

"The Largest Gathering of Numerical Relativists Ever Assembled"

by David Hobill

"Frontiers in Numerical Relativity" was the title of an international workshop that drew more than 60 participants from Canada, Great Britain, France, Israel, South Africa, and Japan as well as from many regions of the United States to Urbana during the week of May 8-13. The meeting, sponsored by NCSA, was without a doubt the largest gathering of numerical relativists ever assembled. Some participants were able to combine their attendance at the conference with a few days working at NCSA's Interdisciplinary Research Center (IRC) before or after the meeting.

That NCSA was able to attract nearly the entire worldwide population of researchers in the field was in large measure due to the high priority the center has placed on research in numerical relativity.



A still image from the videotape of Richard Matzner's numerical simulations investigating the dynamics of cosmic strings. During this interaction, the two strings break and reconnect.

Introduction to Numerical Relativity

As its name implies, numerical relativity concerns the use of numerical methods on the computer for obtaining solutions to the Einstein equations. These coupled nonlinear partial differential equations provide a description of dynamical gravitational fields in general relativity. Since gravity plays a fundamental role in the evolution of astrophysical objects such as stars, galaxies, clusters of galaxies, and even the universe itself, numerical relativity has primarily interested astrophysicists. Some of the phenomena that numerical relativity attempts to understand are the generation and propagation of gravitational radiation, the formation of supernovae, the dynamics of stellar clusters, collisions of neutron stars and black holes, and the behavior of the early universe.

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Visitors at NCSA

Ken Bishop. September 27, 1987–August 1, 1988 from University of Kansas. Area of research: petroleum engineering.

Atsushi Fukada. July 15–August 22 from Nagoya University, Japan. Area of research: history.

Steve Fulling. June 19–July 2 from Texas A&M University. Area of research: mathematics.

Gianni Jacucci. July 7–September 7 from University of Trento, Italy. Area of research: astrophysics.

Margaret Lang. June 21–28 from Tetra Tech Inc. Area of research: forestry.

Mordecai Maclow. May 13–27 and July 7–21 from University of Colorado. Area of research: astrophysics.

Joel Rauber. May 23–August 1 from South Dakota State University. Area of research: astronomy.

Ramesh Sharda. May 23 from Oklahoma State University. Area of research: management science.

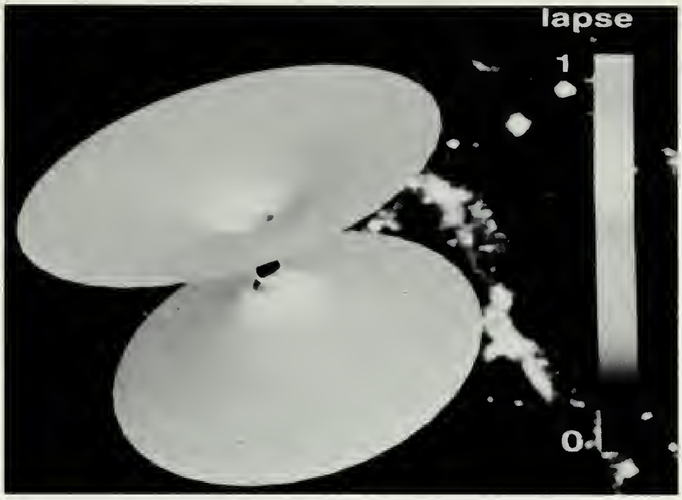
Dean Sumi. June 7–13 from California Institute of Technology. Area of research: astrophysics.

Craig Upson. July 5–10 from Stellar Computer. Area of research: computer animation.

M. Venkataramanan. May 30–June 10 from Indiana University. Area of research: management science.

Phil Yasskin. June 23–27 from Texas A&M University. Area of research: mathematics.

A 3D embedding diagram of a spherically-symmetric black hole. This black-and-white still image was reproduced from a color videotape created at NCSA by David Hobill and David Bernstein.



Relativists *continued from page 1*

Numerical relativity, still considered a fledgling discipline, is barely 10 years old. Although heroic attempts at solving the Einstein equations were made in the late sixties and early seventies, it was not until NCSA Director Larry Smarr (with the help of Kenneth Eppley now at the Stanford Linear Accelerator Center and James Wilson at Lawrence Livermore Natonal Laboratory) was able to solve the problem of two colliding black holes that numerical relativity recorded its first real success.

Now, a decade later, the number of scientists working in this field has grown from less than a handful to almost 100 practitioners. Indeed, the number of researchers in this field has increased twofold in a little over two years. It was not surprising then that approximately 60 percent of the workshop participants were either graduate students or recent Ph.D. recipients.

Also present at the May workshop were many of Dr. Smarr's early collaborators, whose efforts in bringing about the very first numerical solutions of the Einstein equations on a computer are now legendary. This meeting therefore provided one of those rare opportunities for researchers just entering the field to meet and share ideas with those responsible for its creation.

During the five-day conference, 29 talks were given by 38 participants. The fact that a large percentage of the hour-long presentations were shared between two speakers pointed to the importance of collaborative efforts in this particular field.

Workshop Highlights

In opening the conference, Larry Smarr outlined the program currently being pursued at NCSA in computational geometrodynamics, that is, the numerical study of pure gravity. He also discussed the present and future needs of computational scientists and how they would be met through innovations in hardware and software design. The remainder of the first day was dedicated to presentations that discussed various aspects of gravitational collapse in stellar cores and the eventual gravitational radiation produced from such processes. In what may be considered the most ambitious attempt at solving a fully three-dimensional problem, Takashi Nakamura of Kyoto University described his work aimed at determining the dynamics associated with the coalescence of two orbiting neutron stars.

One important problem that arises in almost any physical theory is the description of the interaction between two or more separate bodies. This is particularly difficult in a nonlinear theory such as general relativity. The second day's talks were generally concerned with such problems, and the presentations described the work required to understand collisions of objects that ranged from relativistic heavy nuclei to neutron stars and black holes. While most of these talks dealt with the simpler systems consisting of only two objects, Stuart Shapiro and Saul Teukolsky of Cornell presented their research aimed at understanding the motion of thousands of stars and the eventual formation of clustered stellar systems.

During the following two days a variety of topics were discussed. Tsvi Piran (Hebrew University, Jerusalem) demonstrated under what conditions one might or might not form a "naked singularity" in spacetime through the use of numerical relativity. Other talks covered the development of numerical methods and algorithms that have been used to obtain more accurate and stable results, alternative formalisms of general relativity and their advantages for numerical calculations, the use of finite element methods and smooth particle hydrodynamics, and a number of other technical issues.

The final morning was concerned more with spacetimes that might be used to explore the behavior of the Einstein equations than with solutions that represent physically realistic systems. This is a new development that parallels the analytic work done by more mathematical research. The afternoon sessions dealt with the cosmological issues surrounding the creation of the elements in the early universe and with the interaction of cosmic strings, which may be responsible for the formation of galaxies and clusters of galaxies. The latter presentation, given by Richard Matzner (University of Texas at Austin), included showing what was perhaps the most impressive video shown at this workshop. (Dr. Matzner's videotape was developed with the assistance of Stefen Fangmeier, manager of the NCSA Scientific Visualization Program).

Other Workshop Activities

Extracurricular activities during the conference included two visits to the IRC. One evening was dedicated to a presentation of the different software packages available to NCSA users for

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the visualization of scientific data. Another evening session provided a relaxing view of the different uses of visualization software in such fields as quantum chemistry, fluid dynamics, astrophysics, nonlinear dynamical systems, meteorology, biophysics, and numerical relativity. Joan Centrella (Drexel University) entertained those who attended the conference banquet with a talk that combined humorous reminiscences of her collaborations with Larry Smarr and a discussion of computational scientists' needs for the visualization and analysis of large data sets.

Organizers of the conference were Charles Evans from the California Institute of Technology, L. Samuel Finn from Cornell University, and David Hobill from NCSA. The proceedings, to be published by Cambridge University Press, are expected to be available by the end of the year. ■

Pushing Fractal Frontiers

by Kathleen Robinson

Even those who have learned to read meaning into the mysterious geometry of a fractal aren't sure how to interpret the sometimes disjoint images Dr. Nicholas Kazarinoff has been producing on the NCSA CRAY X-MP/48 supercomputer. A professor of mathematics at State University of New York at Buffalo, Dr. Kazarinoff spent a week in May at the NCSA Interdisciplinary Research Center (IRC) under the auspices of the NCSA Visitors Program, continuing his investigation into "Iterations of Theta Sums."

Dr. Kazarinoff's earlier work in hydrodynamics has led him into the emerging interdisciplinary field of nonlinear dynamics. This field is also known as *chaos* because one focus of the investigations is on the boundary where a system's stability gives way to wild unpredictability. Chaos investigators study the patterns that underlie apparent disorder using recursive calculations and graphic techniques which have been made practical—and in some cases, only possible—by computers.

Mathematicians Become Numerical Experimenters

Historically, the fields of physics and mathematics have been constrained by limitations such as the apparent insolubility of nonlinear equations or the inability of Euclidean geometry to adequately describe the complex shapes that occur in nature. In recent years these limitations have been overcome through the development of numerical experiments that use the computer as the primary research tool—not just for its computational powers, but also for its graphic capabilities. The results of calculations can be displayed in full color on the computer screen where the investigator's intuition and powers of visual exploration can go to work, forming theorems that then can be subjected to the traditional rigors of mathematical proof.

Characteristics of Fractals

One surprising discovery has been that the iterative calculation of relatively simple nonlinear equations can result in multidimensional objects of almost unimaginable complexity. Partly because they may exist in a fractional dimension (hard as that may be to imagine), these objects are called *fractals*. One crucial characteristic shared by fractals is self-similarity. When viewed at many different levels of magnification, fractal objects contain similar degrees of detail and similar shapes. Any one of the spirals, rainbows, wisps, buds, or feathers of a fractal object will be repeated in many scales at different places on that object.

Another characteristic is that the slightest change in a single parameter of the calculation that generates the ultimate image can cause a completely different fractal to appear or cause it to disperse into fractal dust. One focus of nonlinear dynamics research is directed at identifying the types of conditions that bring about such dramatic changes.

Selected Upcoming Meetings

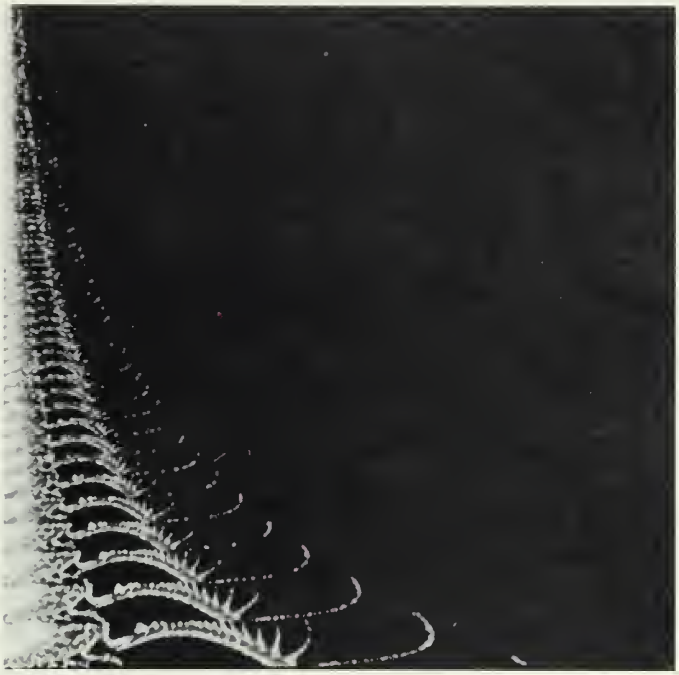
Workshop on UNIX and Supercomputers, September 26–27, 1988, Pittsburgh, Pennsylvania.
For more information, contact Melinda Shore, Pittsburgh Supercomputing Center, 4400 Fifth Avenue, Pittsburgh, PA 15213, (412) 268-5125, `shore@reason.psc.edu`.

Science and Engineering on CRAY Supercomputers, Fourth International Symposium, October 12–14, 1988, Minneapolis, Minnesota.
For more information, contact symposium chairman John E. Aldag, Cray Research Inc., 1333 Northland Drive, Mendota Heights, MN 55120-1095, (612) 681-3646.

Workshop on Practical Iterative Methods for Large-Scale Computations, October 23–25, 1988, University of Minnesota, Minneapolis, Minnesota.
For more information, contact workshop administrator, Angie Vail, Minnesota Supercomputer Institute, 1200 Washington Avenue South, Minneapolis, MN 55415, (612) 624-1356.

Supercomputing '88. November 14–18, 1988. Orlando, Florida.
For more information, contact general chairman George Michael, L-306, Lawrence Livermore National Laboratory, P.O. Box 808, Livermore, CA 94550, (415) 422-4239, `gam@lll-crg.arpa`.

At NCSA Dr. Nicholas Kazarinoff displayed this iteration of the theta function on a complex plane.



Calculations Using the Complex Plane

Fractals like those Dr. Kazarinoff is creating result from repeated calculations that use, for part of their input, a grid of points on the abstract construct that mathematicians call the complex plane. Another important part of the input is the value resulting from the previous level of the computation. The result of each iteration is compared to the boundary of a large disk whose dimensions are established by the investigator.

A pixel on the computer screen is assigned a color according to the number of iterations that occur before the corresponding point on the complex plane exceeds the boundary of the disk. Some points on the complex plane never pass beyond the boundary of the disk. Others pass it quickly on their way, apparently, to infinity. The longer a calculation is run, the more likely it is that the points still within the boundary are there because they never will exceed it, not because they have not yet done so.

Assigning colors to parts of the images is not a trivial part of these investigations. The researcher can enhance some points of information by careful adjustments of the color assignment process. Conversely, some information may be obscured if too gross a color spread is used to represent a range of values.

Working with Theta Functions

Since moving his work from the Macintosh to the CRAY X-MP supercomputer, Dr. Kazarinoff has been using grids on the complex plane ranging from 512 x 512 to 1024 x 1024 points. He suspects, though the images have not yet borne this out, that there may be some points on the complex plane which never move at all when used in certain functional iterations, as well as other points that move in periodic orbits but never leave the chosen boundary. To investigate these ideas, he mathematically maps the coordinates of the computer image onto the coordinates of the grid in the complex plane. The fact that images he has already analyzed do not reveal fixed points may be due sometimes, he feels, to the use of a grid that was not sufficiently fine to trap those points.

The images that result from Dr. Kazarinoff's work are fractals—as demonstrated by the self-similarity they exhibit and their sensitivity to the slightest change in initial conditions—but they have richer (and more confusing) features than have been seen previously. When he magnifies different areas of the structure, bands of repetitive detail appear. As he modifies a single parameter the images undergo dramatic changes, representing bifurcations—another buzzword in the nonlinear dynamics lexicon.

He, for one, is excited rather than put off by the degree of detail. "I'm using a more complicated mathematical function," he says, "so I'm not surprised that the structures seem more complicated." Whereas most calculations previously and currently used to create fractals involve polynomials, or sums of two complex exponentials, the truncated theta function Dr. Kazarinoff is using requires sums of 14 complex exponentials. He settled on that number after some trial and error. "When I used values higher than 14, the numbers were either too large or too small to compute to the necessary precision. I had to take special measures to handle the numbers, and then I couldn't be 100 percent sure the picture I was seeing reflected reality."

Given a fractal's sensitivity to slight changes in parameters, there is some chance that the differences seen in his images may be due to round-off error, rather than being the legitimate result of a more complex calculation. This was a major reason for moving the work to the CRAY X-MP supercomputer. By carrying out the calculations to 63 decimal places, he can place more confidence in the validity of the structures revealed by the computer experiments.

Ongoing Staff Support

Time spent at the IRC this May was actually a return visit for Dr. Kazarinoff, whose several visits totaled about a month here in the spring of 1987. When he left for a lecture tour in China, he took with him about a dozen

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***Frontiers** continued from page 5*

disks of images for further analysis, plus slides and color prints of some of the more spectacular and perplexing formations. Although the work continued long-distance from Buffalo during the academic year, the new image files proved too large for reliable transfer over phone lines.

"We sent him disks of images from time to time," recalls Rick Kufrin, one of the consultants who has been working with Dr. Kazarinoff. Using NCSA Telnet for the Macintosh, Dr. Kazarinoff performed calculations from Buffalo, then phoned the consultants and asked them to describe the resulting pictures so he could try to decide whether he too needed to see them or whether further calculations were needed first.

On-Site Advantages

One of the advantages of doing the work at the IRC, besides the convenience of seeing the pictures firsthand for himself, was the opportunity to focus on the work at hand without the usual workday interruptions. "Dr. Kazarinoff came in here about 10 a.m. and stayed until 2 a.m.," says Michael Welge, a numerical consultant who has worked with him. "That's a *lot* of time on the computer." Reportedly, Dr. Kazarinoff still was running half-hour programs the morning of his scheduled noontime departure.

Steps in a Complicated Process

As for the tools he used, "I think you could call this article 'Dr. Nick Kazarinoff Used ImageTool Like Crazy'," laughed one consultant. "He *really* used it a lot, to fine-tune the color palettes of his images." At the IRC, Dr. Kazarinoff used ImageTool [see ***access*** Vol. 2 No. 1 and 2] on both the Macintosh and the Sun Workstation. However, that was not the starting point of the necessary manipulations.

As an example of the work involved, consider the steps of the process that resulted in a video animation of his 1987 experiments. The results of the calculations were output as raw numbers, which were converted into raster format. Then the hundreds of image files (which ranged in size from .5 megabyte to 1.2 megabytes) were viewed on a Sun Workstation, and different color palettes were applied in an effort to maximize the information conveyed by the image. With the help of the NCSA Scientific Media Services group [SMS—see ***access*** Vol. 2 No. 3], the files were moved to the Alliant FX/80 minisupercomputer. The files were put into the frame buffer, then onto the Abekas A62 digital video storage device, and from there were output as a video animation of the different fractal images.

Musing on Motivation

Asked to explain why he studies fractals, Dr. Kazarinoff had a ready reply. "My own motivation for looking into these complex structures is mathematical curiosity, but simpler fractals have been used by geologists and geographers and astronomers to explain similar physical features in the world around us." He paused to adjust an image on the screen, then added, "We're still applying the mathematics that Isaac Newton did three hundred years ago. The math done today may be used tomorrow, but how far away that tomorrow is, we don't know. One thread connecting studies in contemporary mathematics is the study of patterns—to study patterns seems to be useful. These things have some structure, and sometimes they have poetry or beauty to them as well." Then he turned back to the screen in his visitor's carrel and called up an ImageTool spectrum to show yet another mysteriously beautiful example of just what he meant. ■

Scientific Visualization

Preparations for Siggraph '88

by Veronica Johnston

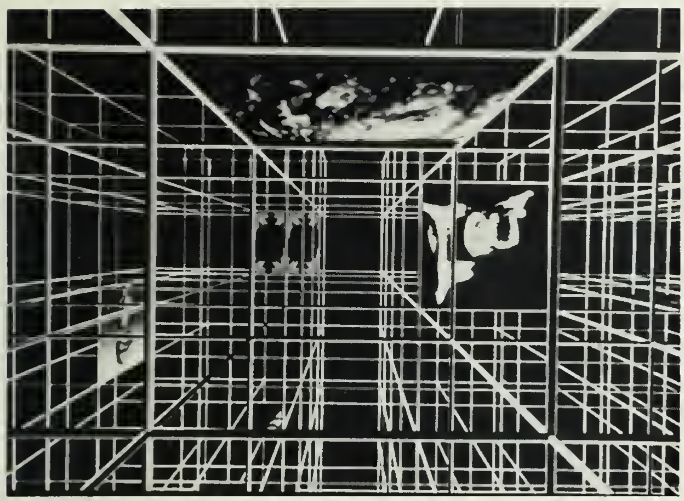
Since November, NCSA staff have been preparing for the 15th Annual Conference on Computer Graphics and Interactive Techniques to be held in Atlanta, Georgia on August 1–5. Sponsored by the Association for Computing Machinery's (ACM) Special Interest Group on Computer Graphics (SIGGRAPH) in cooperation with the Technical Committee on Computer Graphics of the Institute of Electrical and Electronics Engineers Inc. (IEEE), this conference is the largest and most prestigious annual computer graphics conference in the world. SIGGRAPH '87 boasted over 40,000 participants.

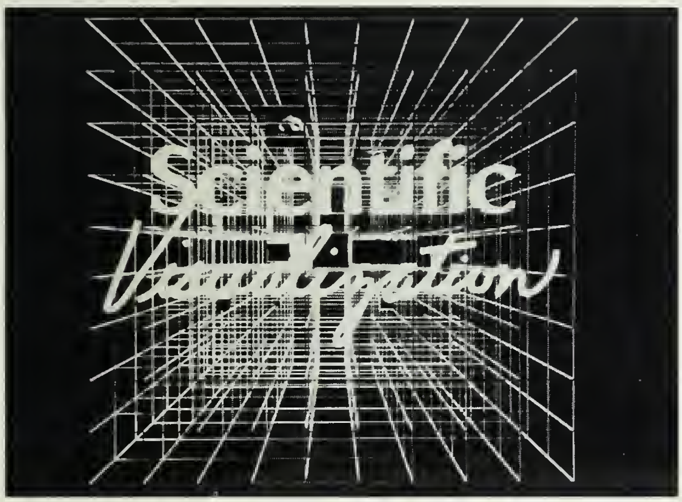
Fifteen NCSA staff members are attending SIGGRAPH '88 to meet with special interest groups and to see panel sessions; courses; film, video, and art shows; hardware and software exhibits; and state-of-the-art visualization technology in the presentation of technical papers.

NCSA Video Selected

The SIGGRAPH film and video show is the world's premiere event of the year for computer graphics animation, and it is an honor to be chosen for the show. This year's show includes a four-minute videotape produced by the NCSA Scientific Visualization Program. Out of 172 entries judged on the basis of technical innovation and creativity in the field of computer graphics, the NCSA visualization video is one of the 40 selected for the film and video show.

Past visualization produced by the center is featured in the framework of a grid in the introduction to this year's NCSA videotape [see photo on next page]. The body of the tape shows the aesthetic highlights of 14 scientific visualization projects produced by NCSA in the last year. These visualization projects, which run from 2 to 12 minutes in their original length, envision large (especially three-dimensional) supercomputer data sets of scientific research from astrophysics, chemistry, geophysics, and biology. Scientists use visualization





Upper Left A still image from the introduction of the NCSA videotape. The grid represents a scientific computational domain.

Lower Left Software developed at NCSA for the visualization of scientific data created the text in this image. *Scientific* was generated with a program that calculates contour surfaces for volumetric data and *visualization* with a generalized cylinder program.

Above Donna Cox, UIUC professor of art and design and NCSA visiting faculty, was honored in June when she was elected by the ACM membership to serve on the SIGGRAPH Executive Committee. [This photo first appeared on the cover of ***access***, Vol. 1 No. 3.]

to both understand their data and communicate their findings to their peers.

All the featured visualization pieces as well as the tape's introduction were produced using the Scientific Visualization Program's production software: a Wavefront Technologies Inc. package and in-house software developed for data filtering and object modeling. In the title sequence of the videotape, the NCSA-developed software forms the word *scientific* and writes the word *visualization*. This same software models complex three-dimensional data sets in most of the scientific segments.

As at SIGGRAPH '87 [see ***access***, Vol. 1 No. 3], the NCSA videotape is also being shown at the booths of Wavefront Technologies Inc. and Alliant Computer Systems Corporation. Wavefront software and an Alliant FX/80 form the backbone of the NCSA Scientific Visualization Program.

Additional NCSA Participation

Three NCSA staff are lecturing or chairing panel discussions at SIGGRAPH '88:

- Robert Haber, group leader of the RIVERS project [Research on Interactive Visual EnviRonmentS—see ***access*** Vol. 2 No. 3] and NCSA adjunct professor of supercomputing applications, chairs the panel "Hardware Strategies for Scientific Visualization" and lectures in the "Visualization Techniques in the Physical Sciences" course.
- Stefen Fangmeier, Scientific Visualization Program manager, lectures in the "Computer Graphics in Science" course.
- Donna Cox, University of Illinois at Urbana-Champaign (UIUC) professor of art and design as well as visiting faculty at NCSA, lectures in the Educators Workshop entitled "Collaboration in Computer Graphics Education."

"SIGGRAPH is an important forum for the exchange of ideas related to computer graphics," said Stefen Fangmeier. "One attends this conference to learn from what others are doing in the field, to share insights with peers, and to be inspired." He added, "All the extra hours late at night and on weekends we put into producing our SIGGRAPH submission will pay off 100 percent when we see those images on the big screen along with thousands of people who appreciate the effort and its outcome." ■

NCSA Industrial Program Is on the Move

by Larry White

A bold endeavor is underway at the National Center for Supercomputing Applications to bring new techniques, new algorithms, and new technologies to leading corporate research centers in America. This endeavor, the NCSA Industrial Program, is proceeding under the broad vision of Larry Smarr, director of NCSA, to integrate the best researchers from corporate America into the fabric of the Interdisciplinary Research Center (IRC) at NCSA. This partnership, built on new cooperation among government, industry, and academia toward a unifying goal, aims to strengthen America's international competitiveness.

Left to right: Larry White and John Stevenson, both of the NCSA Industrial Program, welcome Motorola researcher Randall Luneack.

John Stevenson, who has over 25 years experience in the Bell telephone system, is the NCSA Associate Director responsible for the NCSA Industrial Program. Mr. Stevenson's strong leadership and marketing skills guide NCSA in reaching those leaders in major American corporations who have the insight to understand what partnership with NCSA can bring to each company, and he possesses the talent and skills to develop those partnerships.

The tools of computational science provide a new methodology for the study of the complex systems around us. These tools—supercomputers, high-powered visualization capability, and networked personal graphics workstations—provide scientists with new insights into the world around us. With the right application of these tools, corporate researchers can develop better products at less expense and bring them to market earlier. These tools fill the increasingly sophisticated needs corporate scientists have in today's marketplace of international competition, product liability, and consumer awareness.

Using the supercomputer and its distributed environment, corporate researchers can perform experiments on the computer with realistic complexity. Researchers can model the biological activity of molecules and conduct research on photographic chemistry, oil chemistry, electronic components, economic theories, mechanical or hydraulic systems, and optical systems. By using the supercomputer to simulate new products with realistic complexity before spending money on expensive prototypes, researchers can produce better products at less expense and in shorter time.

Types of Industrial Programs

Full Partnerships. NCSA, with its IRC, provides a unique environment for corporate researchers to interact with their academic colleagues. Corporate scientists, university faculty, and visiting researchers collaborate to develop basic research techniques, algorithms, and applications. Full partnership in the NCSA Industrial Program allows corporate researchers to immerse themselves in the unique advanced computing environment of people and facilities provided by the IRC.

Full partners in the NCSA Industrial Program receive extensive training on using and managing supercomputing systems, access to advanced workstations and software, the services of the visualization group, and resources for performing their own proprietary research. Industrial participants benefit from and participate in the ongoing development of tomorrow's computational environment. Full partnership in the NCSA Industrial Program requires a substantial financial commitment by the corporation over a minimum of three years, allowing NCSA to accomplish long-range planning and to acquire resources for the program.

Eastman Kodak Inc. became the first full partner in the NCSA Industrial Program in August 1986 and has been affiliated long enough to reap benefits from the program. Kodak's management carefully documents the many ways that supercomputing creates cost-effective progress in their research efforts. More recent partners—Amoco Corporation, Eli Lilly and Company, and Motorola Inc.—are building momentum in the program by identifying projects, software applications, and the people they would like to have participate in the center and by having their participants receive advanced training from NCSA. Other corporations, not yet partners in the program, are in various stages of evaluating their potential membership.

Associate Partnerships. Associate partnership in the NCSA Industrial Program exposes corporations to benefits of supercomputing at a lower level of commitment than that required from full partners. Associate partnerships, although only recently announced [see ***access***, Vol. 2 No. 2], have attracted considerable interest from many corporations that would like to evaluate the potential of supercomputing and visualization by working on a significant research project here at the center. Exposure to supercomputing in this program benefits the corporation not only with direct computational results, but also in its understanding of the impact that new computational technology will have on its research.

Vendor Relationships. NCSA seeks out relationships with leading technology vendors of computing hardware and software, networking equipment and services, and other tools of computational science. These relationships provide the vendors with a neutral, innovative computational environment in which to evaluate their product offerings, to determine requirements for their future product offerings, and to participate in the development of tomorrow's comprehensive computational facility.

These relationships, in turn, provide both NCSA and its industrial partners with access to the latest equipment from these technology vendors—sometimes equipment that is not yet available in the marketplace. Such advance exposure helps the NCSA and its partners in their development and long-range planning activities.

Future Directions for NCSA–Industry Relations

The NCSA Industrial Program is continuing to design new programs and to enhance existing programs as it brings together the best minds in both corporate and academic research. Strengthening American corporate competitiveness, supporting academic research, and progressing toward tomorrow's comprehensive computational facilities are all major benefits we will achieve. ■

What Can the NCSA Academic Affiliates Program Do for You?

by Alan Craig

Through the NCSA Academic Affiliates Program, NCSA brings supercomputing resources to the national research community at college and university campuses across the nation. An affiliate campus enters a mutually beneficial relationship with NCSA. There are currently more than 60 NCSA academic affiliate campuses.

Affiliate campuses enjoy a number of benefits, including:

- a block grant of time on the NCSA CRAY X-MP/48 supercomputer. This block grant is used at the discretion of the affiliate campus for user and consultant training, exploration, graduate and undergraduate classes, and quick startup of research projects.
- training for affiliate contact people. NCSA currently offers two phases of training: basic (Phase I) and advanced (Phase II).
- help in accessing NCSA via national networks.
- both written and online documentation for computer systems available at NCSA.
- the "inside scoop" on NCSA activities.

All universities and colleges interested in supporting supercomputing researchers on their campuses are eligible to join the NCSA Academic Affiliates Program. There are no fees, but NCSA does expect an affiliate campus to:

- send a contact person to NCSA Affiliate Training Sessions.
- provide on-site consulting to their local supercomputer users.
- provide training sessions on their campus for local researchers.
- send periodic reports to NCSA describing what the affiliate contact and local supercomputer users are doing.

For more information about the NCSA Academic Affiliates Program or to learn how to become an affiliate campus, telephone Alan Craig at (217) 244-1988 or send electronic mail to BITNET address `13020@ncsavmsa` or to Internet address `acraig@ncsaa.ncsa.edu`. ■

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Duke University
Shiangtai Tuan
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Eastern Illinois University
Dave Henard
(217) 581-3227
Gallaudet University
Donald V. Torr
(202) 651-5027
George Washington University
Thomas E. Moyer
(202) 944-6389
Georgia Institute of Technology
Mary Trauner
(404) 894-6166
Harvard University
Lewis Law
(617) 495-2627
Illinois Institute of Technology
Patrick Feldner
(312) 567-5962
Indiana University
Robert Holden
(812) 335-9258
Kansas State University
Neil Erdwein
(913) 532-6311
New Mexico State University
Joseph R. Denk
(505) 646-3439
New York University
Jeff Bary
(212) 998-3049
North Dakota State University
Mark Gordon
(701) 237-8011
Northern Illinois University
Samnuan Duramad
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Northwestern University
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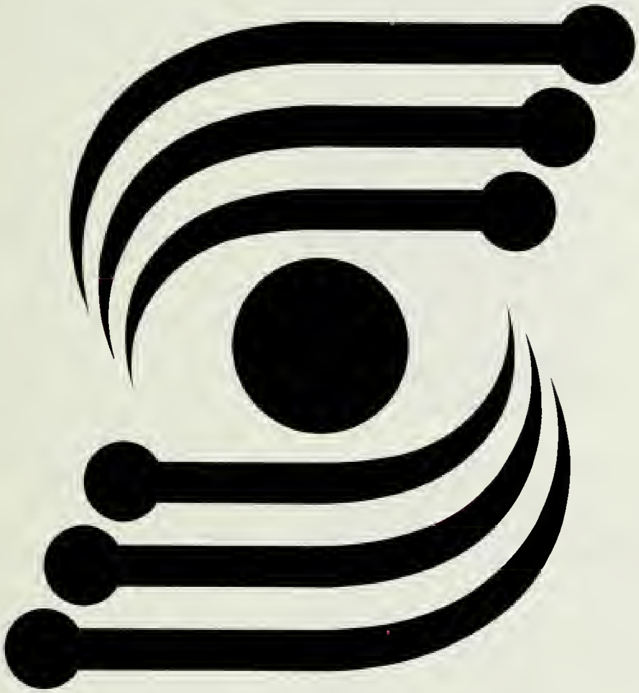
New Look for NCSA Materials

by Mary Hoffman

This issue of ***access*** marks the official inauguration of the NCSA logo, centerpiece of the center's new comprehensive visual identity program.

Selected by Director Larry Smarr, Deputy Director Jim Bottum, and Associate Director Harriett Weatherford, the new logo brings together the diverse aspects and applications of the center and serves to visually promote NCSA as a world-class scientific institute.



About the Logo

In addition to being a striking visual image, the logo has a symbolic component. The circle represents NCSA's strategic position in the supercomputer community, and the curving lines represent the arrays of communications networks of interdependent centers throughout the world. The design can stand alone or be incorporated as the *S* in NCSA.

The interaction of the circle and the curving projections comprise a dynamic structure, providing a graphic image that suggests the potential for explosive growth in the supercomputing industry.

About the Artist

The logo and layout were designed by Roman Duszek, Polish scholar and artist with international experience. Recent entries in Professor Duszek's portfolio include the Lot Air (the Polish national airline) and Warsaw subway system logos. Currently he is a Visiting Professor of Graphic Design in the College of Fine and Applied Arts at UIUC.

About the Visual Identity Program

The new NCSA visual identity program is comprehensive and will be applied across four major areas:

- publications (documentation, public relations fliers, and reports)
- signage that falls outside UIUC visual identity guidelines
- video materials (training and public relations videotapes, scientific animation tapes, 35mm slides, and transparencies)
- exhibition displays

Using a coordinated image across these areas will provide a visually unified framework for all of the center's activities.

The new visual identity program has the capacity to expand as the needs of NCSA expand and change. Please address any questions or comments to Melissa Johnson, Manager, Documentation and Publications, National Center for Supercomputing Applications, 605 East Springfield Avenue, Champaign, IL 61820. ■

Parallel Processing and Numerical Applications

by William Allen

A Numerical Applications Seminar held at NCSA May 5–6 marks the beginning of a parallel-processing initiative in which scientists and computer manufacturers are cooperating to find the best forms of parallel computing.

Approximately 75 people from universities and the private sector attended the NCSA-sponsored seminar. It featured a wide range of talks on such subjects as design of parallel algorithms, multitasking, and architecture for parallel computations. Speakers came from Argonne National Laboratory (ANL), the Center for Supercomputing Research and Development (CSRD), the UIUC Department of Computer Science, NCSA, Alliant Computer Systems Corporation, Cray Research Inc., and Myrias Computer Systems Inc.

Above Four speakers chat between sessions. Left to right: Michael Berry of the Center for Supercomputing Research and Development (CSRD), Martin Walker of Myrias Computer Systems Inc., Richard Foster (back to camera) of Myrias, and Jack Perry of Alliant Computer Systems Corporation.

Right John Larson of Cray Research Inc. discussed multitasking on the CRAY-2 supercomputing system.

"This meeting represents the first major thrust of NCSA into the world of alternative architectures for advanced scientific computing machines, software, and applications," said Michael Welge, numerical consultant at the center and organizer of the seminar. Such seminars allow researchers to investigate the possibilities of new machines and help couple the research community with vendors in evaluating future development.

"We are promoting parallel computation," Mr. Welge said. "Most scientists believe the future of scientific computing is in parallel processing. We need new languages, algorithms, and hardware. This gathering is just a start."

Larry Smarr, NCSA director, said that the scientific community is in the "preinfancy" of parallel computing and predicted that the next few years should produce developments as exciting as any in the past four decades of computing. He noted that UIUC's combined strengths of CSRD, NCSA, and the Department of Computer Science offer the campus tremendous potential for exploring parallel computing. The growing relationship with ANL also will play a significant role.

The CRAY-2 supercomputer, scheduled to arrive at NCSA in the fall, will join the CRAY X-MP/48, Alliant FX/8, and Alliant FX/80 systems already in-house. Dr. Smarr said the NCSA five-year plan calls for acquiring a CRAY-3, and the center also may obtain other systems with advanced architectures in the near future.

"NCSA must become a 'garden of architectures,'" Dr. Smarr said. "As a national center, it is essential that we develop access to a wide variety of architectures for scientists and engineers to experiment with."

Mr. Welge said a second seminar on numerical applications is being planned for next spring. ■

The 1988 NCSA Summer Institute

by Scott Lathrop

The NCSA 1988 Summer Institute was held June 6–17 at the center. For three years NCSA has held a summer institute to provide two weeks of intensive training on the use of supercomputers. This year's topics included:

- network access to NCSA facilities
- how to use both the CTSS and UNICOS operating systems
- how to use the Alliant system
- introduction to hardware for both the CRAY X-MP and CRAY-2 computer systems
- vectorization and optimization on a CRAY supercomputer
- multitasking on Alliant and CRAY systems
- numerical libraries
- graphics
- experiences of various scientists using supercomputers in their own fields of research

Upper Right Fifty researchers attended the 1988 NCSA Summer Institute.

This year's NCSA Summer Institute provided funding for 25 researchers to attend the two-week session. An additional 25 observers were invited to attend the institute at their own expense. NSF provided the major funding. Cray Research Inc. generously funded three participants. NCSA received over 100 applications for this year's institute.

Institutions represented at the 1988 NCSA Summer Institute included:

University of Iowa
Indiana University
University of California at Santa Barbara
Columbia University
Iowa State University
University of Washington
Texas A&M University
Illinois Institute of Technology
Northwestern University
Rennselaer Polytechnic Institute
North Dakota State University
Notre Dame University
South Dakota State University
University of Missouri at Rolla
University of Massachusetts
Colorado State University
University of Illinois at Urbana-Champaign
Argonne National Laboratory

Staff from NCSA industrial partners also attended the institute.

The summer institute is a valuable program that allows researchers to receive in-depth training from both NCSA staff and outside experts. Comments (including the samples at left) indicate that this year's NCSA Summer Institute was extremely beneficial to the participants. ■

Comments on the 1988 NCSA Summer Institute—

"The facilities at NCSA are top rate and the staff is more than willing to share their knowledge, experience, and equipment."

"It is very rare that a conference lives up to one's hopeful expectations; this institute has."

"I expect that my attendance here will facilitate my work in the near future to a great extent."

"I felt that the staff at NCSA went out of their way to make our stay more comfortable and productive. They are very concerned about helping each individual obtain the maximum benefit from the institute."

"The summer institute was very professional and had very state-of-the-art equipment and software."

"People were great and so was the organization."

A New Building for Interdisciplinary Research at UIUC

by Fran Bond

Recently NCSA staff donned hard hats to tour the Arnold O. and Mabel M. Beckman Institute for Advanced Science and Technology. Funds for constructing this institute on the UIUC campus—$40 million, the largest monetary gift to a public university to date—were donated by alumni Mr. and Mrs. Beckman to provide office, laboratory, and meeting space for interdisciplinary research. Some groups within NCSA, such as the Computational Science Program, are expected to occupy space in the Beckman Institute.

As seen in the photo (right), most of the exterior work is finished. The main entrance, a tower, was inspired by the Italian *campanile* (bell tower) form. Detroit architects Smith, Hinchman, & Grylls Associates Inc. designed the building in a modification of the contemporary PostModern style, with traditional details adapted from a number of historical periods. NCSA is slated to occupy parts in four floors of the H-shaped building. An atrium connects both halves of the structure.

To continue the design of UIUC's main campus, a landscaped quad is planned for the area occupied by the vehicles and trailers in the photograph.

Look for more news of NCSA and the Beckman Institute in future issues of ***access***. ■

Above The Beckman Institute, showing the south facade of the nearly completed exterior, with the girders of the *campanile* (bell tower) exposed. The building is scheduled to be occupied by January 1989.

Left NCSA assistant directors Mike Smith (Operations) and Scott Lathrop (User Services) visit the site of the Institute under construction. The UIUC campus is in the background.

UNICOS Is Coming

by Stephanie Drake

NCSA is adopting UNICOS as the operating system for the CRAY-2 and CRAY X-MP/48 supercomputers. We believe that this change will enable us to provide better service to our users.

The CRAY-2 supercomputer will be installed this fall with the UNICOS operating system. Planning is underway for the phased-in transition from CTSS to UNICOS on the CRAY X-MP supercomputer. Current plans call for the transition to begin in the first quarter of calendar year 1989 and to be completed within three months.

UNICOS is supplied by Cray Research Inc. (CRI) and is based on AT&T System V UNIX.

The decision to change operating systems was based on many considerations, including input from researchers through NCSA user surveys, advisory groups, and personal contacts; the desirability of a vendor-supported operating system and of a transparent path from workstation to supercomputer; reduced training needed by researchers already familiar with UNIX on their own workstations; capabilities available in UNICOS that are not available in the baseline version of CTSS, such as multitasking, quick release of CRI-supplied compilers and utilities, windowing systems, NFS (Network File System), and enhanced batch job submittal.

If you have any questions or comments concerning the move to UNICOS, please send electronic mail to BITNET address `13007@ncsavmsa` or to Internet address `13007@ncsaa.ncsa.uiuc.edu` or telephone David McWilliams at (217) 244-0640. ■

Fortran Standards Committee Meets at UIUC

by Kurt W. Hirchert

During the week of May 9–13, NCSA hosted a meeting of X3J3, the technical committee responsible for the ANSI Fortran standard. Since 1978, when the current standard was adopted, X3J3 has been working on a revision of the standard. In October 1987, a draft of the revision was released for public comment (see ***access***, Vol. 1 No. 5), with the public comment period ending in February 1988. The UIUC meeting was the first since the close of the public comment period.

The draft provided many new features, including source form extensions, more flexible memory management, array-valued expressions and assignment, user-defined types, more portable selection of REAL and COMPLEX representations, intrinsics to determine the properties of the REAL and COMPLEX representations, internal procedures, procedure and operator overloading, recursion, an enhanced procedure interface, and a facility for global sharing of data that is independent of storage association.

The draft did not lack supporters, but the majority of comments received by the committee expressed sentiments ranging from concern to ardent opposition. The most prevalent theme was that the revised language was too large and complex. Ironically, however, many of the same comments expressed displeasure at the absence of pointers, bit manipulation facilities, or a standard textual inclusion capability.

At the May meeting, there was much discussion of how to modify the draft to address the public comments. Although the two-thirds majority needed to change the draft was mustered on a number of specific issues (such as the addition of a textual inclusion capability), no consensus was reached on the extent to which the proposed language would need to be cut back to satisfy the concerns about language complexity. Positions ranged from a belief that the resulting language should be closer to FORTRAN 77 than the current draft (that is, that more than half of the new features should be dropped) to a belief that very little could be removed from the current draft without having a serious negative impact on the ability of Fortran to adequately support the expanding needs of scientific computing.

Because many of the features in the current draft are interrelated, the committee felt that isolated consideration of individual features would be inappropriate. Accordingly, several groups of committee members volunteered to independently prepare comprehensive plans for changes to the proposed language. These competing plans will be presented at the next X3J3 meeting, to be held in Jackson Hole, Wyoming during the second week of August.

If you would like further information, you may contact X3J3 committee member and NCSA consultant Kurt Hirchert by using the Internet address hirchert@ncsa.uiuc.edu. ■

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ARPANET Problems (SRI-Network Information Center)	(800) 235-3155 (415) 859-3695 nic@sri-nic.arpa

NCSA Applications Software Emphasis

by Scott Lathrop

As part of the NCSA commitment to make available appropriate applications software, the NCSA Applications Software Group has identified key areas of concentration. You may contact the coordinators below to learn more about software plans at NCSA and to give direct input to the software process.

Area of Concentration	**Coordinator**	**Telephone**
Astronomical Image Processing System	Radha Nandkumar	(217) 244-0650
Benchmarking	Beth Richardson	(217) 333-6276
Chemistry	Harrell Sellers	(217) 333-2754
Computational Fluid Dynamics	Mark Johnson	(217) 244-0643
Engineering (finite element analysis, nuclear engineering)	Ilhan Dilber	(217) 244-1973
Electrical Engineering	Mark Straka	(217) 244-1991
Graphics	Mike Krogh	(217) 333-0166
Mathematics	Beth Richardson	(217) 333-6276
Parallel Methods	Michael Welge	(217) 244-1999
Symbolic Manipulation	Steve Christensen	(217) 244-0544
Systems Utilities	Doru Marcusiu	(217) 244-1334
Workstations	Joseph Hardin	(217) 244-6095

These are the people to contact for suggestions about software that you would like to see on the NCSA systems. Please inform the coordinator of your concerns and interests in a particular area of concentration.

Other areas of concentration are receiving attention and will be highlighted in the future. Please direct your general comments to Brand Fortner, Manager, Applications Software Group, by telephoning (217) 244-1347 or by sending electronic mail to BITNET address `14007@ncsavmsa` or to Internet address `fortner@ncsa.ncsa.uiuc.edu` or to AppleLink address `A0162`. ■

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Important Dos and Don'ts with Batch Jobs

by Shyam Duggirala, Ilhan Dilber, and Doru Marcusiu

This article lists a series of important precautions you should follow to preserve the integrity of your programs when using the batch system on the CRAY X-MP/48 supercomputer.

MSC/NASTRAN Engineering Software Now Available

by Ramesh Jayaraman

Now available on the CRAY X-MP/48 supercomputer, MSC/NASTRAN is a proprietary general purpose program capable of solving a wide variety of engineering field problems.

NCSALIB Expanded

by Mark Straka

Four new routines for converting between CRAY and IEEE floating point formats have been added to NCSALIB on the CRAY X-MP/48 supercomputer.

Precision Visuals Software Installed

by Mike Krogh

FORTRAN-callable libraries from Precision Visuals Inc. that provide a device independent graphics system have recently been installed on several NCSA systems including the MicroVAXes, Suns, Alliants, and the CRAY X-MP/48 supercomputer.

Setting a Forwarding Address in VAX Mail

by David McWilliams

Since many users only log on to NCSA VAX computers to check for electronic mail, this article explains how to set a forwarding address in VMS mail to have mail sent automatically to your home system.

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access
the NCSA newsletter

September–October 1988 vol. 2 no. 5

Science

Large-Scale Computation in Semiconductor Physics

by Kathleen Robinson

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Dr. Karl Hess, recently appointed Associate Director of the Beckman Institute at UIUC, heads a group studying complex problems in compound semiconductor research.

Dr. Karl Hess, recently appointed an Associate Director of the Beckman Institute at UIUC [see ***access*** July–August 1988], has been involved with NCSA since the center's earliest days. He and his colleagues use the NCSA CRAY X-MP/48 supercomputer to develop simulation methods in many areas of solid state electronics.

The outstanding problems are so complex that progress can be made only by using large computational resources. Even with the speed of the CRAY X-MP computer, they need 20 minutes of supercomputer time to calculate what happens in a semiconductor in just 10 nanoseconds (10 billionth of a second).

According to Dr. Hess, "The advent of very large scale integration as well as new developments in compound semiconductor research have opened new horizons. The complexity of systems and the speed of components are growing at an astonishing pace."

Novel Semiconductor Devices

One branch of research being undertaken by Dr. Hess's group investigates new semiconductor devices that use novel structures and materials. Until recently, most semiconductor devices were made from silicon. Recent development in the field of semiconductor physics concentrates on compounds such as gallium arsenide and on artificial crystals (superlattices). These structures offer new opportunities due to quantum effects such as resonant tunneling that Dr. Hess and his group are actively investigating using several methods, including real-time Feynman path integrals.

Improved Semiconductor Laser Design

Another branch of their research relates to the development of the first computer-aided design (CAD) program for simulating and optimizing the design of semiconductor lasers. Properties that can be designed and optimized include light intensity, heat distribution, switching speed, and expected lifetime. Light intensity is sometimes more important than length of expected service. On the other hand, unequal heat distribution affects the lifetime of a device, so if a device needs to last a long time, distributing the heat evenly will be important to the designer. Dr. Hess and his group are working to develop a robust and user-friendly system for designing and optimizing these devices.

Semiconductors *continued on page 3*

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An Apology

The atom exchange simulation cited in May-June ***access*** was run by Paul Bash and Martin Field, both of Harvard University, on the CRAY-2 system at the Minnesota Supercomputing Center. We regret that we neglected to mention the Minnesota center in that article.

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***Semiconductors** continued from page 1*

Conventional and Monte Carlo Simulations

In yet another set of projects, Dr. Hess and his group are simulating conventional devices made of silicon to study effects that occur when a device is reduced in size. One reason for making smaller devices is to increase their speed: the shorter the distance an electron must travel, the faster the device. However, the electrons gain very high energies, and this changes the properties of the circuit.

Silicon has been used for years and its properties are well known, but when it began to be used on a microscopic scale perplexing results were observed. When silicon components were relatively large, quantum effects arising from the device size could be ignored. As smaller semiconductors have been designed, it has become necessary to take into account the device size and to think of electrons as moving through a matrix of atoms, rather than across a plane of homogeneous material. Quantum effects and nonlinearities arising from the high electric fields must therefore be considered. Dr. Hess's group has developed Monte Carlo particle simulations that include all the complications of nonequilibrium statistics and the properties of electrons at high energies.

Dynamic Views

Dr. Hess and his group have found that new methods for visualizing experimental results are becoming more and more important. Dr. Umberto Ravaioli, who recently joined Dr. Hess's group at UIUC, has been focusing on methods for graphically representing the results of their experiments, in addition to his other research interests. Says Dr. Ravaioli, “We are trying to develop a number of specific visualizing tools for our area. Right now we are working on a three-dimensional simulator to represent electrons in momentum space. Visualization is very important when the supercomputer generates an enormous amount of data in a short time. In many cases, a video is the best way to analyze the results or to show them in a conference.”

In other cases, significant discoveries have resulted from insights gained through visual analysis of data. One surprising discovery the group made is that most transistors switch *off* faster than they switch *on*. This fact was not previously known, but was obvious once they were able to watch the flow of electrons through a device. Subsequent experiments suggested by this visual discovery have substantiated the finding. Another phenomenon clearly visible is the “turbulent” motion of electrons through materials. This observed turbulence has implications for understanding the boundary conditions which heavily influence the behavior of semiconducting devices.

Changing Approaches

“Our approach to science and engineering problems has changed qualitatively and quantitatively in several significant ways,” says Dr. Hess. He identifies two sources of these changes: the availability of the CRAY supercomputer to academic researchers and increased interaction among disciplines.

Dr. Hess and his research group have a new attitude toward education and self-education. Instead of working only with other researchers in physical electronics, they now work regularly with faculty and students in physics, electrical engineering, and computer science.

Another new approach relates to ideas and algorithms previously considered too complex. Says Dr. Hess, “We have developed a basic confidence to approach problems which are just barely possible to solve with the fastest computers, and we know that these algorithms will have broad use as widely available computational resources improve at a rapid pace.”

New Horizons in Electronics

Dr. Hess believes that the use of quantum interference phenomena in nanostructures, and the possibility of constructing wave guides for electronics, will open new horizons in electronics for making novel ultrafast integrated circuits. Prepared by their recent experiences and using their new approach, Dr. Hess and his research group will be in the forefront, developing the methods for a quantitative understanding of a new research area. §

New—Electronic Mailing List on Relativity

A directory of scientists, mathematicians, and others interested in the theories of special and general relativity and related fields is being established to improve electronic communication worldwide.

This effort is being organized by Malcolm MacCallum at Queen Mary College in London, England. Steve Christensen, NCSA research scientist, is collecting addresses in the U.S. to forward to Dr. MacCallum.

If you or someone at your institution would like to be on this electronic mailing list, please email the following information to Dr. Christensen. If you have more than one possible address, send them all. Please be as complete as possible.

- **full name**
- **address**
- **interests (optional)**
- **email addresses**
- **telephone**
- **computers and software used (optional)**

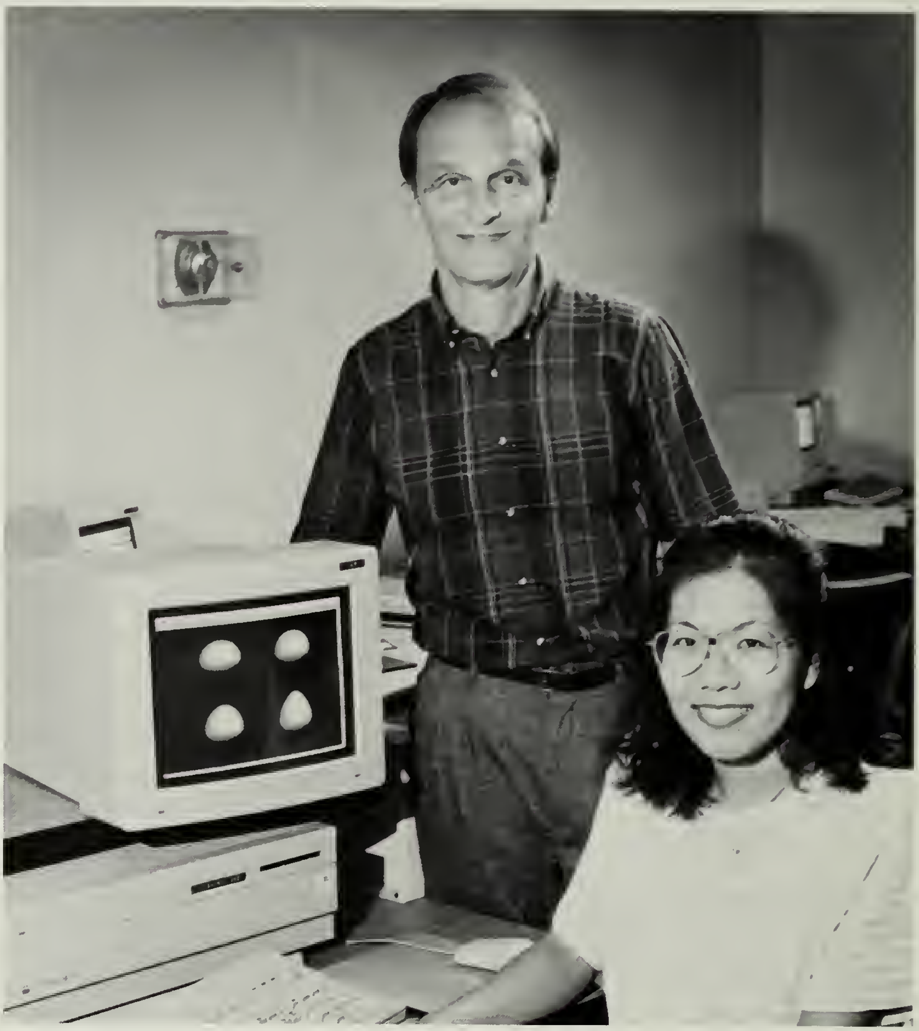
Steve Christensen's electronic mail addresses are:

steve@ncsa.uiuc.edu (Internet)
14008@ncsavmsa (BITNET)

Dr. Christensen will acknowledge each mailing list request to verify that the links are working. If you receive no acknowledgement in a few days, please resend your email message or send the information via regular mail.

"Raindrops Keep Falling" in the CRAY

by Dan Leonard



Kenneth V. Beard and Cathy Chuang demonstrate raindrop shapes they have reconstructed by simulating on the supercomputer natural forces acting on the drops.

Despite this summer's drought, raindrops have continued to fall in the NCSA CRAY X-MP/48 supercomputer as scientists attempt to discover the secrets of drop shape and to help cure some of the problems rainstorms create for the communications industry.

Kenneth V. Beard, professor of meteorology at UIUC, and Cathy Chuang, graduate research assistant at the Illinois State Water Survey, are using the CRAY supercomputer to reconstruct the shape of a raindrop based on forces acting on it in nature. They hope that this and other basic research into the nature of raindrops will someday be used to improve radar estimates of rainfall rate and help solve the problem of cross talk in telephone connections.

Raindrops and Radar Signals

Patches of rain scatter radar signals, allowing meteorologists to determine how hard it is raining. The severity of this scattering depends on the size of the raindrops in the storm.

"If you are trying to estimate how hard it is raining, you've got to know the concentration of large drops, because they are the ones that contribute most of the radar backscattering and most of the rainfall rate," Dr. Beard said.

Raindrops and Communication Signals

Rainstorms also interfere with transmission of microwave communication signals, such as telephone conversations. To fit more channels into a given frequency range, adjacent signals have different polarizations, he explained. As the signal passes through a rainstorm, it is depolarized by the raindrops. As a result, a receiver tuned to one frequency may pick up traces of the signal on a neighboring channel. Background voices during telephone conversations are an example of this cross talk phenomenon.

A "rain outage" occurs when the signal is so deteriorated by the raindrops that it is completely lost in a rainstorm, Dr. Beard said. In this case, no microwave can successfully pass through the storm.

Determining the exact shape of raindrops will enable other scientists to better estimate the amount of depolarization occurring in a storm.

Modeling Raindrops

Drag Forces. The first mathematical model of the raindrop constructed by Dr. Beard and Ms. Chuang was based solely on the aerodynamic drag forces produced as the drop falls through the air. Using a VAX 11/780 minicomputer, they reconstructed the shape of a drop using theoretical drag forces.

The simulated shape did not at all resemble a teardrop, the raindrop shape popularized by animators and advertisers. It looked more like a hamburger bun falling flat side down. This calculated shape corresponded well with images of actual raindrops recorded by other scientists in the past.

Electric Fields. But drag forces alone do not accurately model all raindrops. For example, drops found in thunderstorms pass through strong electric fields generated by the storm. These forces needed to be added to the model.

In spring 1987, Ms. Chuang used the NCSA CRAY X-MP computer to calculate raindrop shape under the forces of the electric field alone. After validifying this simulation by comparing it with laboratory observations, Ms. Chuang updated the model to combine the electric field forces and aerodynamic forces, producing an even more nearly accurate model for the shape of a raindrop in a thunderstorm.

Static Electric Charge. Dr. Beard and Ms. Chuang were still not finished with the raindrop simulation. In addition to passing through a storm's electric fields, a raindrop usually possesses a static electric charge of its own. The electric field and the static charge produce a repellent force that slows the fall of the drop. Some small drops even become stationary in midair as the repellent forces negate the pull of gravity.

In most cases, however, the repellent force simply slows down the drop. The reduced velocity changes the drag force, which in turn changes the drop shape as well as the influence of other forces on the drop shape.

Using their earlier research method, Dr. Beard and Ms. Chuang began by modeling the simpler case of a charged drop falling in the absence of an electric field. They found that because the static charge reduces the surface tension of the drop, aerodynamic drag forces distort the drop more.

As a final step, all the forces studied so far—aerodynamic drag, electric field, static charge, and gravity—were combined in the supercomputer model to produce the most accurate picture of a raindrop to date.

From the Supercomputer to the Tropics

In the spring of 1989, Dr. Beard plans to return to Hilo, Hawaii. There, in 1985, he and his colleagues discovered some of the world's largest raindrops while flying through thick rain shafts over the Pacific Ocean. He hopes to validate the latest model of the drop shape by gathering additional information on the size and shape of the large raindrops in the heavy rains in this tropical setting. §

Long-Term Visitor Models Black Holes

by Kathleen Robinson and David Hobill

Joel Rauber, assistant professor of physics at South Dakota State University, spent the summer at the NCSA Interdisciplinary Research Center (IRC) under the auspices of the cen-ter's Visitors Program. This was Dr. Rauber's third summer at NCSA, making him one of the few long-term visitors whose associations with the IRC predate the Visitors Program. In May, he also visited NCSA as a participant in the Frontiers of Numerical Relativity workshop [see ***access***, July–August 1988], which attracted numerical relativists throughout the world to Champaign-Urbana.

Dr. Rauber has been using the CRAY X-MP/48 supercomputer to help construct solutions to the equations that determine the initial configuration of two colliding black holes. Visiting NCSA has enabled him to interact with the center's director, Larry Smarr, and graduate student David Bernstein and postdoctoral research fellow David Hobill, who are developing codes that will calculate the dynamics of black holes.

The results of Dr. Rauber's work will provide the starting point for subsequent computations that will calculate the dynamics of colliding black holes and the gravitational radiation generated during that process.

Several difficulties are associated with the problems Dr. Rauber is trying to solve. First, arbitrary values cannot be assigned to all of the functions and parameters that determine the initial configuration of two black holes. The number of initial datasets possible are restricted by a subset of the Einstein equations that describe the behavior of the gravitational field. Second, since the governing equations are coupled nonlinear partial differential equations, solving them is not a trivial matter. Finally, these equations must be solved with great accuracy to ensure that the resulting evolution obtained through computer simulations is not hampered by the propagation of numerical errors contained in the initial data.

Joel Rauber, assistant professor of physics at South Dakota State University.

The first case Dr. Rauber is tackling is that of two spinning black holes whose axes of rotation are aligned along the direction of their intended motion. When the two black holes are spinning in opposite directions—a configuration Dr. Smarr calls the "cosmic screw"—the collision is expected to produce some spectacular results. Once this scenario has been modeled successfully, Dr. Rauber expects to expand his research efforts to a wider range of configurations, namely any number of black holes, all with different rates of rotation.

Why Black Holes?

A black hole is a region in both space and time from which no information (including light) can escape due to the strength of its gravitational field. Most black holes are thought to result from the collapse of sufficiently large stars that have exhausted their nuclear fuel. Others may have been produced during the Big Bang, the explosive event that created our universe. Still others may issue from collisions of large numbers of closely packed stars.

Long-Term Visitor *continued on page 6*

Long-Term Visitor continued from page 5

As early as 200 years ago, the idea of an object that prevents light from escaping was discussed by Laplace using Newton's theory of gravity. But not until 1916—when Karl Schwarzschild constructed a solution to the spherically symmetric Einstein equations—was the modern concept of a black hole begun. However, even though the mathematical solution existed, confusion reigned over its physical interpretation. The term *black hole* was not applied and the true physical nature of these objects was not understood until the 1960s after Roy Kerr discovered a solution representing a rotating black hole in 1963.

During the past fifteen years astronomers have discovered a number of candidates for black holes, and controversy still continues over whether or not these objects *are* black holes. Although the existence of black holes may still be shrouded in mystery, theoreticians in general relativity find them interesting because they represent bodies made up purely of gravitational fields. As such, they are the simplest objects that can be described by Einstein's theory of gravity.

Since gravity is so weak that any measurement of its relativistic effects requires the observation of very massive objects available only in astrophysical systems, black holes have a special appeal. The dynamics of black holes can supply important information concerning the differences between the Newtonian and the Einsteinian theories of gravity—without having to deal with the internal constitution of planets, stars, and galaxies. This is why Dr. Rauber and his colleagues study the dynamics of black holes.

Early attempts to describe the dynamical behavior of black holes used purely mathematical analysis, but these failed due to the nonlinear nature of the systems being studied. In the late 1970s, Dr. Smarr and his coworkers were the first researchers to successfully use computers in the calculation of the head-on collision between two nonrotating black holes.

The initial data Dr. Rauber generates will be used by still other researchers to calculate more general collisions involving charged black holes, rotating black holes, and any number of black holes moving in different directions. Some of these calculations will have to wait for the development of faster and more powerful supercomputers before they can even be attempted.

Expanded Research Opportunities

Dr. Rauber's work at the IRC is partially supported by a Research at Undergraduate Institutions (RUI) grant from NSF. Summers are his only opportunity for a concentrated research effort.

The Visitors Program has made it possible for Dr. Rauber to work at the IRC, an opportunity for invaluable scientific and technical contacts with other visitors and NCSA staff. Interacting with other researchers doing numerical work has been very helpful.

Working at the IRC also has enabled Dr. Rauber to mix and match math libraries—something impossible at his own university because their few math libraries are scattered in laboratories all over the campus. One math package he learned about at the IRC that has been quite useful in his work is PCGPAK, which uses an iterative conjugant gradient method for solving systems of linear algebraic equations.

Asked whether he has been generating too much data to assimilate easily, Dr. Rauber laughs. "That *would* be a nice change," he says. "Right now I have very little in the way of showy results. Eventually, though, I expect I'll need the help of the visualization group here." §

Scientific Visitors at NCSA

Sergio Corvetta. August 1–25 from Office of Industry, Provence Bolzano, Italy. Area of research: economic aspects in computer science of manufacturing.

Iori Emilio. August 9–31 from University of Parma, Italy. Area of research: quantitative physics/artificial intelligence.

Atsushi Fukada. July 15–August 22 from Nagoya University, Japan. Area of research: history.

Phil Hardee. July 12–22 from University of Alabama at Tuscaloosa. Area of research: astrophysics.

Gianni Jacucci. July 7–September 7 from University of Trento, Italy. Area of research: quantitative and computational physics/artificial intelligence.

Jeffrey R. Kuhn. August 29–31 from Michigan State University. Area of research: astrophysics.

Ngee Lek. July 11–August 31. Area of research: power systems.

Mary White. July 11–12 from Center for Wetland Research, Louisiana State University. Area of research: biotic systems.

Computational Science at NCSA

by Stephanie Drake

The NCSA Computational Science Program is coordinated by Associate Director Michael Norman [second from right in photo below]. An internationally recognized astrophysicist, Dr. Norman is frequently cited for his pioneering computational studies of fluid flows. His reputation attracts collaborators from around the world to NCSA.

In front of the CRAY X-MP/48 supercomputer. Left to right: John Stevenson (associate director, Industrial Program); Jim Bottum (deputy director and acting associate director, Systems and Services); Larry Smarr (director), Michael Norman (associate director, Computational Science Program); and Harriett Weatherford (associate director, Finance and Administration).

Creating a Pool of Research Scientists

Since its inception NCSA has had scientists on staff—in addition to Director Larry Smarr—to pursue their own computational research and to lend advice to other scientists using the supercomputing facilities at the center. As Dr. Norman says, "Each scientist uses the unique opportunities at NCSA to accomplish his or her own research projects."

It is impossible to have on staff a scientist in every research area, so the center draws on the talents and interests of the outstanding UIUC research faculty by helping support a number of collaborative, superthrust projects with professors in such areas as civil engineering, astronomical imaging, genome sequencing analysis, protein structure, medical science, urban and regional planning, agriculture, psychology—and the list continues to grow.

The Computational Science Program also works with the center's industrial partners to further industrial research.

Focusing on Research Scientists

Five research scientists are on staff at NCSA, and the center is advertising for a sixth—a computational biomolecular scientist. The role of an NCSA research scientist is multidimensional: he or she conducts original computational research, maintains national and international collaborations, serves as an NCSA spokesperson, participates in center committees, helps develop new technology and software, and provides in-depth scientific consulting.

This article initiates an ***access*** series that will profile NCSA research scientists, associate research scientists, research associates, and adjunct research faculty. Here is a brief introduction, in alphabetical order, to the five research scientists at NCSA.

David Ceperley—quantum statistical mechanics. A worldwide expert in quantum many-body systems, Dr. Ceperley has been developing and applying quantum simulation methods. He has collaborated nationally and internationally in the development of electronic structure methods and has served as a resource person in condensed matter physics and Monte Carlo techniques to study many-body systems such as electrons in metals and solids.

Steven Christensen—quantum gravity. Dr. Christensen is the focal point for symbolic computing [see page 3 and ***access*** May–June 1988]. He has formed an 80-member Sun User Group and is president of the Mathematica user group. Mathematica (developed

Computational Science continued on page 8

Computational Science continued from page 7

by Dr. Stephen Wolfram of Wolfram Research Inc., Champaign) couples a symbolic manipulation package with a sophisticated graphical interface that will, according to Dr. Norman, "open the eyes of all computational scientists."

Barbara Mihalas—radiation transport. In addition to her research in radiation hydrodynamics, Dr. Mihalas has been defining and developing a prototype data management facility. Dr. Norman explains, "There's not a computational scientist alive who doesn't have a data management problem." The data management facility has the potential to radically affect researchers in every discipline.

Michael Norman—numerical astrophysics and gas dynamics. The project that excites Dr. Norman right now is ZEUS code development, a community application software for astrophysical fluid dynamics. Dr. Norman readily admits that at the moment his research is being carried forward by his collaborators and students. He also developed ImageTool for the Sun Workstation [see ***access*** May–June 1988] and is a coordinator of the Santa Barbara ITP Workshop on Computational Fluid Dynamics, which will run from September 1988 through January 1989.

Robert Wilhelmson—atmospheric sciences. Dr. Wilhelmson is "leading the charge in applying parallel algorithms to the general area of computational fluid dynamics," according to Dr. Norman [see ***access*** September–October 1987]. Since his problems are three-dimensional, he has been forced to be resourceful in his code design. Dr. Wilhelmson has been the first NCSA scientist to experiment with multitasking and microtasking on a CRAY-2 supercomputer.

Other Researchers

Associate research scientists such as Roger Ove, research associates such as David Hobill, and NCSA adjunct faculty also will be profiled in this series. Adjunct faculty includes such outstanding UIUC academic researchers as:

- Roy Campbell—computer science—who, along with NCSA's Charlie Catlett, has just received a substantial grant from AT & T to research and implement switched 56 Kbps networking [see ***access*** May–June 1988]

- Josef Cohen—psychology—who has formulated the first truly rigorous theory of color

- Donna Cox—art and design—who has recently been elected to the SIGGRAPH board of directors and often lectures on her concept of Renaissance teams [see ***access*** May–June and July–August 1988]

- Richard Crutcher—astronomy

- Robert Haber—civil engineering—who is heading the RIVERS project [see ***access*** May–June 1988]

- Frank Wrestler and David Lawrence—medicine

What's Ahead?

NCSA has a very clear mission:

To use the tools and techniques of leading-edge computational science to contribute to advances in science and engineering and to strengthen the competitiveness of American industry.

To help the center carry out its mission, the Computational Science Program has established its own five-point goals of:

- Supporting outstanding computational science research
- Promoting a computational approach in new disciplines
- Fostering collaborative interdisciplinary research
- Developing and distributing improved software tools
- Prototyping advanced computational systems

Through the in-house expertise of scientists, the local strengths of UIUC faculty and students, coordination with other laboratories and agencies, and cooperative projects with strategic vendors, the NCSA Computational Science Program will carry forward the NCSA mission. §

Center Activities

UNICOS Update

by Mary Hoffman

NCSA is proceeding with its migration to the UNICOS operating system on its CRAY supercomputers [see ***access*** July–August 1988]. The migration plan calls for installation of the new CRAY-2 system running UNICOS and conversion of all users on the CRAY X-MP system to UNICOS.

A 20-page preparatory manual, the *UNICOS Migration Plan*, was mailed to all users in late August and is also available in online CRAY X-MP and VAX help files (enter `help migration`). If you did not receive the printed document, please call NCSA at (217) 244-0072 and request a copy.

Call for Friendly Users

If you are interested in becoming a friendly user (on either the CRAY-2 system or the CRAY X-MP/48 system under UNICOS), please contact Scott Lathrop by sending electronic mail to 13006@ncsavmsa (BITNET) or to 13006@ncsaa.ncsa.uiuc.edu (Internet) or by telephoning (217) 244-1099.

These friendly user periods are to help "shake out the bugs" in the new systems. We are looking for a small group of users who will be in touch often to let us know of any problems or concerns. The friendly user test periods are not intended for stable production work.

Both friendly user test periods are expected to begin in November.

Migration Timeline

NCSA staff will experiment with UNICOS on the CRAY X-MP/48 system during daily specified test times between August and November 1988. The CRAY-2 system is now scheduled to arrive the first of November.

Full production on the CRAY-2 system is expected to begin in January 1989, just days before the formal transition period begins on the CRAY

X-MP system. During the formal transition period, both UNICOS and CTSS will run on the X-MP system at separate times each day. The UNICOS portion of time will increase up to full production in April 1989.

See the timeline at right for more details. All dates in this timeline are subject to change.

UNICOS migration timeline. All dates are subject to change. You can find the most up-to-date timeline in the Migration help files on both the CRAY X-MP and VAX systems.

November 1988

- November 1 deadline for CRAY-2 proposals for December PRB or SAC review [see page 10]
- CRAY-2 system arrives—estimated four-week installation
- *UNICOS Migration Guide* is mailed to all users
- UNICOS Training begins
- Friendly user access to CRAY X-MP/UNICOS system begins
- Friendly user access to CRAY-2 system begins

December 1988

- PRB or SAC reviews and allocates initial set of CRAY-2 projects as well as CRAY X-MP projects

January 1989

- CRAY-2 system runs UNICOS in full production
- CRAY X-MP/UNICOS transition begins

April 1989

- CRAY X-MP system runs UNICOS in full production
- CTSS removed

Training and Documentation

NCSA is offering training sessions to help you port code and get started with UNICOS. [See the training schedule on page 11 for dates and registration information.]

Pertinent UNICOS documentation produced by Cray Research Inc. may be ordered from the online catalog [see page 19]. Additional UNICOS documentation will be included in the catalog as it becomes available. For more information on UNICOS documentation, contact the Documentation and Publications group [see **NCSA Contacts**, page 23].

Applications Software

All applications packages currently running under CTSS will be available on at least one of the two CRAY systems during and after the transition. [See applications software lists on pages 20–22.] It is not financially or, in many cases, operationally feasible to run all applications on both machines.

Conversion Can Begin Now

We recommend that you begin the conversion process as soon as possible. FORTRAN code modification can be done now in the CTSS environment, and other file conversion processes can be completed during the three-month transition period starting in January.

If you will be continuing your work on the CRAY X-MP computer under the UNICOS operating system, files that you move from the CTSS to the UNICOS environment must be converted to the proper format. NCSA is developing utilities for you to use in this conversion.

Both during and after the transitional phase, the NCSA consulting staff will help you solve problems you may experience in moving files between the two operating systems.

New FORTRAN Compiler

An important part of the migration to UNICOS is that a new FORTRAN compiler is being recommended. Cray Research Inc. has selected the CFT77 FORTRAN compiler for all future work and development.

NCSA has provided a version of the CFT77 compiler under CTSS (enter `help cft77`) so that you can modify your codes before the operating system changeover takes place. You can then invoke the ckcft utility to check for library calls that are included in CFTLIB, NCSALIB, and FORTLIB—none of which will be available under UNICOS. This utility checks only for explicit subroutine calls. Function calls will appear as unresolved externals when loading.

The existing CFT compiler will be available on the CRAY X-MP system under UNICOS, but not on the CRAY-2 system.

Use Notesfiles for More Information

So that NCSA staff and users can share experiences during the transition, we have set up VAX machines ncsavmsa and ncsavmsb for notesfile computer conferencing. Notesfiles will be an especially useful resource during the transition.

The use of notesfiles is included in the migration plan and in this issue of ***data link***, which also gives a complete list of notes conferences.

Updated information will continue to appear in ***access*** and will be incorporated into a UNICOS migration guide which we will send to all users in November.

If you have questions or concerns that cannot be resolved in the notesfiles, please contact the Consulting Office [see **NCSA Contacts**, page 23].

We want to work with you to minimize the impact on your scientific work. If you require extended assistance, contact Dave McWilliams, manager of Systems Consultants, to arrange for a consultant to work with you through your conversion. Contact him by telephoning (217) 244-0640 or by sending electronic mail to 13007@ncsavmsa (BITNET) or to 13007@ncsaa.ncsa.uiuc.edu (Internet). §

Allocation Procedures and Policies for the CRAY-2 and CRAY X-MP/48 Systems

by Patricia Wenzel

If you are interested in applying for time on either the CRAY-2 or the CRAY X-MP/48 computer system, please read this article carefully. We will keep you informed as procedures or policies are amended to better serve your needs.

CRAY-2 Allocations

The current UNICOS migration plan calls for the CRAY-2 system to be available to friendly users chosen by NCSA during a shakedown in November and December 1988. Reviewed and allocated projects will be added to the machine early in 1989.

If you are interested in becoming a friendly user on the CRAY-2 system, please send email to Scott Lathrop, Assistant Director for User Services (see phone number and electronic mail addresses at the end of this article).

During the shakedown, *friendly* will indeed be the key word to describe our friendly users because:

- the system will not be stable
- software will be sparse
- software changes will occur often
- downtimes will be frequent
- hours of access will be limited

Users with current allocations on the CRAY X-MP system may request that some or all of their allocations be moved to the CRAY-2 system when production begins. [See page 11 for details.]

Comparing the Two Supercomputer Systems

Technical Features

CRAY X-MP System

memory in megawords (MW)

- 8 MW total
- 3 MW user limit during weekdays
- 6.5 MW user limit on weekends

operating system

- CTSS until April 1989
  (migration to UNICOS begins January 1989)

CRAY-2 System

memory in megawords (MW)

- 128 MW total
- weekday and weekend memory limits under discussion

operating system

- UNICOS
  (Cray Research Inc. version of AT&T System V UNIX)

Criteria for Using Each System

CRAY X-MP System

- intrinsic merit of the research
- relevance of the research
- research performance competence
- effect of the research on the infrastructure of science and engineering
- demonstrated need for a supercomputer

CRAY-2 System

- all criteria for the X-MP system plus the following
- required ≥ 3 MW of memory
- probability of using the multitasking capability
- availability of software

Policies

The operating policies for the two systems are different and may change as we gain experience with both systems.

CRAY X-MP System

- no dedicated time
- at the expiration date, 25 percent of unused service units may be carried forward for a maximum of six months, if the principal investigator has submitted a letter of justification

service units (SU) charges for academic users

- priority*(.8*CPU+.2*mem residency)

CRAY-2 System

- a researcher may ask to use the entire machine during "dedicated time" (to be used for multitasking; criteria and application procedures for dedicated time are still being formulated)
- no extensions will be granted

service units (SU) charges for academic users

- .8*CPU+(.2*mem residency/16)

Memory residency is measured in MW hours. For those using multitasking on the CRAY-2 system, memory residency will be averaged over the number of simultaneous processors in use.

The charging algorithms are subject to change based upon the experience we will gain with the hardware, operating systems, and demand for resources.

Software. Software available on the CRAY X-MP/48 system may not be available on the CRAY-2 system, and vice versa. Please refer to the software lists on page 20.

Application, Review, and Allocation

November 1, 1988 is the deadline for submitting applications for time on both the CRAY-2 and CRAY X-MP systems. To get an up-to-date applications packet, contact New Accounts/ Users [see **NCSA Contacts**, page 23].

Applications received by the November 1 deadline will be considered either by the joint NCSA/Pittsburgh Supercomputer Center Peer Review Board (PRB) at its December 1988 meeting or by the internal NCSA Small Allocation Committee (SAC).

If you currently have an allocation on the CRAY X-MP system and would like to move all or part of it to the CRAY-2 system, you must write a letter indicating how many SUs of your current allocation you would like to move and justifying your need for the CRAY-2 system. Your request will be reviewed by SAC. Future allocations on the CRAY-2 system will be reviewed and allocated as enumerated below.

Standard procedures for reviewing proposals and allocating time will be the same for both systems, as follows:

1a. Proposals of 100 or more SUs will be reviewed by the PRB, which meets quarterly in March, June, September and December. Applications must be received by the first of the month (about 6 weeks) before each meeting to allow time for review. Deadlines are February 1, May 1, August 1, and November 1.

1b. Proposals of 6–100 SUs will be reviewed externally and allocated by SAC, which meets monthly. Lead time for these proposals is 6–8 weeks to allow time for external review.

1c. Start-up grant proposals of 5 or fewer SUs will be allocated by SAC without external review. Lead time for these proposals is two to four weeks. A proposal received two weeks before the next SAC meeting can be reviewed at that meeting.

2. The same application form will be used for both the CRAY X-MP and CRAY-2 systems.

3. Multiyear proposals will be accepted, with time in the out years based on an annual progress report submitted by the principle investigator and the availability of CPU cycles.

4. A proposal may include applications for either or both systems. You must indicate which system you are applying for, state how many SUs you are requesting for each system, and justify the need for the system based on the criteria listed in this article.

Contacts for Friendly Users and for Allocation Process

Scott Lathrop
Assistant Director, User Services
telephone: (217) 244-1099
BITNET: 13006@ncsavmsa
Internet: 13006@ncsaa.ncsa.uiuc.edu

Patricia Wenzel
Manager, User Administration
telephone: (217) 244-0074
BITNET: wenzel@ncsavmsa
Internet: wenzel@ncsaa.ncsa.uiuc.edu
§

Training Sessions for New Supercomputer Users

by Alan Craig

Due to the transition from CTSS to UNICOS, NCSA will offer its final two-day CTSS training session in October. Thereafter, NCSA training will be directed at helping both migrating users and new users get started with UNICOS. The UNICOS New User Training sessions will be three-and-a-half days long. Enrollment is limited.

1988	
October 3,4	Final CTSS New User Training
November 28–December 1	UNICOS Friendly User Training
December 5–9	UNICOS Training for Academic Affiliates
1989	
January 9–12	UNICOS New User Training
January 23–26	UNICOS New User Training
February 20–23	UNICOS New User Training
March 6–10	UNICOS Training for Academic Affiliates
March 20–23	UNICOS New User Training
April 17–20	UNICOS New User Training

You must have a CRAY userid to register, and you must register at least one week before the session. To register for a training session or to get more information about the training program, please contact the NCSA Training Program [see **NCSA Contacts**, page 23]. To see the latest training schedule, enter `help training` on the VAX or CRAY computer.

If you would like to extend your visit at NCSA beyond the training program dates, contact the NCSA Visitors Program [see **NCSA Contacts**, page 23].

First Undergraduate Employee Scholarship Awarded

by Joseph Hardin

Gaige Paulsen, student programmer and first recipient of the NCSA Undergraduate Employee Scholarship Award.

Nearly 20 undergraduate students work at NCSA and help keep the center going. NCSA recently established the Undergraduate Employee Scholarship Award to recognize outstanding efforts by undergraduate staff.

This award recognizes distinguished service to the goals and mission of NCSA—work that has contributed to efforts that have won NCSA national recognition or distinguished NCSA as an institution of excellence. The award provides tuition and fees at UIUC.

The first recipient of this award—Gaige Paulsen—sets a high standard for those to come.

Gaige, currently a student programmer in the Software Development Group, has been programming at NCSA since November 1985. This December, after three and a half years of undergraduate study, he will receive his BS in engineering computer science.

Along with workstation programmer Tim Krauskopf, he is one of the authors of NCSA Telnet. Gaige is the primary author of the Macintosh version of this incredibly successful software program.

NCSA Telnet for the Macintosh

NCSA Telnet for the Macintosh allows Macintosh computers to communicate with any host that can use the TCP/IP protocol suite. These computers range from CRAY X-MP and IBM 3090 computers to Sun Workstations and MicroVAX computers. Using currently available Ethernet and AppleTalk hardware along with NCSA Telnet, a Mac can be connected simultaneously to up to 20 different machines for terminal emulation and file transfer.

Begun two years ago, in the fall of 1986, the Telnet project at NCSA has reached international proportions and garnered considerable praise from the networking community. Cited in national magazines such as *MacWeek, MacWorld, Macintosh Today, MacUser,* and *Computer and Communications DECISIONS*, NCSA Telnet has made a significant media impact.

In addition to being cited in magazine articles, Telnet is mentioned in the Black Box network catalog (with a complete citation of NCSA and the University of Illinois) as one of the features of their Black Box FastPath; both Kinetics and Cayman Systems are shipping NCSA Telnet with their networking products; and Apple Computer Inc. has mentioned NCSA Telnet in its *Desktop Communications Solutions Reference Guide.*

Telnet Use Worldwide

Each day between 10,000 and 20,000 people in the United States and more than 1,000 in Great Britain use NCSA Telnet. An additional example of its widespread acceptance is that it is used by the entire Finnish supercomputing network.

Although many original users of NCSA Telnet were in the academic community (demonstrated by the fact that over 80 universities downloaded the newest release in the first two weeks of its availability), the industrial community has expressed growing interest. To date, we know of user communities at Boeing, General Electric, NeXT, Apple Computer, Dow Chemical, Motorola, DuPont, John Deere, Bell Northern Research, Cray Research, Hewlett-Packard, Claris, and other firms. In addition, all major NASA sites are using NCSA Telnet.

Telnet is used in development work at yet other institutions. Ford Aerospace has chosen to use NCSA Telnet as a testing ground for the Space Station Environment, which they are developing for NASA. Brown University has produced a program, known as TN3270 for the Macintosh, that allows Macintosh computers to communicate easily with IBM mainframes. TN3270 uses NCSA Telnet as the basis for its communications.

Good Work, Gaige!

The NCSA Telnet project has been an excellent bearer of goodwill for the center. It is definitely one of the most successful projects to come out of the NCSA Workstation Group, which has evolved into the Software Development Group.

It's hard to imagine a more exciting success story than NCSA Telnet, but we're sure that Gaige will come up with one.

Congratulations, Gaige, from all your colleagues at NCSA! §

A Record-Setting NCSA/PSC Peer Review Board Meeting

by Patricia Wenzel

The joint NCSA/PSC Peer Review Board (PRB) met June 23, 1988 at Urbana.

Records Are Set

The board set a new record for the number of proposals reviewed in a single meeting: 48 proposals. Twenty-eight of these proposals were from the Pittsburgh Supercomputing Center.

Several additional records were set for NCSA proposals and service units (SUs) reviewed at a PRB meeting:

largest number of proposals:	20
most service units requested:	11,112
most service units allocated:	6,437

NCSA continues to carry a backlog of allocations that are being added to the system as old accounts expire. This queue of excess demand is now about three months long. Most of the SUs allocated at the PRB meeting have been added to the queue.

Guidelines for Writing Proposals

Members of the PRB stressed that the guidelines on the NSF allocation form number 1235 should be adhered to when writing a proposal. The board has been rejecting proposals that do not follow these guidelines.

NCSA has revised its instructions for completing an application and now provides a sample proposal that the PRB classified as "excellent!" Before submitting your next proposal please contact New Accounts/Users [see **NCSA Contacts**, page 23] to obtain an up-to-date application packet.

Board Changes

Wayne Hendrickson (Biochemistry and Molecular Biophysics), Columbia University, has stepped down from the board. Ralph Roskies (PSC Director) and Mike Norman (NCSA Associate Director for Computational Science) are working together to find a replacement in Dr. Hendrickson's area of expertise.

The next PRB meeting will be held in September. §

Supercomputing and Molecular Modeling Attract Industry and Academia to Workshop

by Robert Goldstein
University of Illinois at Chicago

Researchers from various oil, pharmaceutical, and computer companies recently met at the Computer Center of the University of Illinois at Chicago (UIC) for the first week-long UIC Supercomputer User Workshop.

The pilot workshop, sponsored jointly by the UIC Computer Center and NCSA, focused on the evaluation and parameterization of force fields in molecular modeling. That this is a question of more than academic interest was demonstrated by the participation of such companies as Amoco Corporation, Eli Lilly and Company, Eastman Kodak, ETA, IBM, Parke-Davis, and Allied Signal.

Two themes central to the UIC supercomputing education program [see ***access*** May–June 1988] ran throughout the workshop: how best to use supercomputers and how best to use software (molecular modeling software, in this case).

Both themes were discussed in morning lectures by T. J. O'Donnell (NCSA), Nora Sabelli (UIC), Robert Goldstein (UIC), George Pack (UIC–Rockford), Ron Elber (UIC), Jim Snyder (Searle), Steve Roy (UIC), Scott Kahn (UIUC), and Shashi Rao (Searle). The afternoons were devoted to hands-on calculations, using both supercomputers and local workstations.

In addition to the mainframe computers in the UIC Computer Center, participants had access to supercomputers at NCSA, Cornell, and the University of Georgia. Control Data Corporation provided time on the ETA 10P at Georgia and allowed UIC the use of three CDC 910-300 high-end workstations.

Evans and Sutherland donated the use of three of their workstations and the computers necessary to run them. These types of graphically oriented workstations have become necessary to understand the results of massive calculations for molecular images. Of course, the workstations are useless without software to draw easily manipulated images; the necessary software was loaned to UIC by Tripos Associates and by Polygen Inc.

Although exercises were planned around calculations on the unusual antibiotic ristocetin, many participants brought along their own problems and were eager to continue calculating after the daily formal sessions ended.

The success of this workshop will hopefully result in a continuing program to bring together industry and academia at the University of Illinois. §

Illinois Pre-engineering and Science Educators Meet at Center

by Alan Craig

Above Howard Wakeland, associate dean for student affairs in the College of Engineering, addresses a workshop luncheon.

Right Larry Smarr, director of NCSA, speaks with one of the workshop participants during a break.

On July 14 and 15, the UIUC College of Engineering Office of Continuing Education and NCSA jointly hosted a workshop entitled, An Overview of Supercomputing for Illinois Pre-Engineering and Science Educators.

Twenty-two instructors from educational institutions throughout the state gathered at NCSA. The two-day workshop provided a broad overview of what supercomputing is all about and what is going on at NCSA in particular.

Dr. Larry Smarr, NCSA director, opened the workshop. He spoke of computational science and the need for supercomputing. Dr. Michael Norman, NCSA associate director for computational science, described some of the science being done at NCSA and the computational science process. [See page 7 for a profile of the Computational Science Program.] Both speakers emphasized the need for scientific visualization as well as other tools and techniques being explored at the center.

Topics of other talks included distributed computing, vectorization and parallel processing, and the NCSA Academic Affiliates program. UIUC professor Donna Cox gave a multimedia presentation entitled "Renaissance Teams and Supercomputer Graphics: A Convergence of Art and Science" [see ***access*** July–August 1988]. Howard Wakeland, associate dean of the College of Engineering, and Dr. Robert Bender, director of the UIUC Office of Public Service, also addressed the group.

During lab sessions, participants could try the CRAY X-MP/48 supercomputer firsthand.

Illinois community and four-year colleges and universities represented at the workshop included:

Blackhawk College
College of Lake County
Harold Washington College
Harper College
Highland College
Illinois Central College
Illinois State University
Illinois Valley Community College
Lincoln Trail College
Moraine Valley Community College
Parkland College
Richland College §

NCSA User's Group Meeting—October 17 & 18

by Janice Knapp-Cordes

The first annual NCSA User's Group Meeting will be held Monday and Tuesday, October 17 and 18, 1988, at Jumer's Castle Lodge in Urbana, Illinois.

Why a User's Group Meeting?

The User's Group Meeting is being held to:

- update users on the center's progress and plans for the future
- get input from NCSA users
- enable users and staff to interact

Users who attend will receive a report on the scientific impact of NCSA. In addition, several NCSA staff will update users on hardware, software, visualization, networking, training, and documentation. Two Academic Affiliate sites will report on their experiences. Parallel working sessions on the second day will focus on user questions and input.

Who Should Attend?

All users of NCSA computing facilities are invited and urged to attend. Serving our user community is a primary goal of NCSA, and we can best do this with significant input from users.

Attendees are asked to send in their questions, comments, and suggestions before the meeting so that the issues can be addressed thoroughly.

To register for the meeting, please call (217) 333-2883 by September 30 and ask for Joanie Chenoweth, program secretary. If you will be paying your own way, you must provide your social security number; billing an organization requires a FEIN number. The $85 registration fee covers all meals Monday as well as breakfast and lunch Tuesday. A no meals $50 registration fee is also available.

You must make your own room reservations. Please call Jumer's at (800) 525-8637 and identify yourself as part of the NCSA User's Group Meeting.

Register today! §

NCSA to Host International Colloquium in December

by Stephanie Drake

Supercomputing in Atomic Physics is the title of a colloquium open to researchers in physics, astronomy, chemistry, geology, and engineering who are interested in ab initio calculations of the optical properties (photoionization cross sections as well as line strengths and profiles) of atoms. The colloquium will be held at NCSA on December 21, 1988 and is sponsored jointly by the United States/United Kingdom Opacity Group and NCSA.

The colloquium follows two days of scientific and technical meetings of some of the world's experts in computational atomic physics. These researchers, who compose the Opacity Group, are carrying out comprehensive calculations for a new set of astrophysical opacities, primarily in stellar envelopes. Several of the group members will be addressing the colloquium on December 21.

NCSA research consultant Dimitri Mihalas is organizing the December meetings. To register for the colloquium, please contact Dr. Mihalas by telephoning (217) 333-5529 or by sending electronic mail to 15001@ncsavmsa (BITNET) or to 15001@ncsaa.ncsa.uiuc.edu (Internet). There is no registration fee for the colloquium, but space is limited. §

Selected Upcoming Meetings

Workshop on Practical Iterative Methods for Large-Scale Computations, October 23–25, 1988.University of Minnesota, Minneapolis, Minnesota.
For more information, contact workshop administrator, Angie Vail, Minnesota Supercomputer Institute, 1200 Washington Avenue South, Minneapolis, MN 55415, (612) 624-1356.

Supercomputing '88. November 14–18, 1988. Orlando, Florida.
For more information, contact general chairman George Michael, L-306, Lawrence Livermore National Laboratory, P.O. Box 808, Livermore, CA 94550, (415) 422-4239, gam@lll-crg.arpa.

Supercomputers, Hypercubes, and High Performance Architectures, course 169.
October 25–28, Boston; November 22–25, Ottawa; December 6–9, Washington, DC; February 21–24, Los Angeles; February 28–March 3, Washington, DC; March 7–10, Boston. For more information, contact Integrated Computer Systems, (800) 421-8166.

Image Processing and Machine Vision, course 411.
October 25–28, Ottawa; November 1–4, Los Angeles; November 29–December 2, San Diego; December 6–9, Washington, DC; February 21–24, Los Angeles. For more information, contact Integrated Computer Systems, (800) 421-8166.

Computer Graphics: Software Techniques and Hardware Components, course 365.
November 1–4, Washington, DC; November 15–18, Toronto; November 29–December 2, Los Angeles; February 14–17, Washington, DC; February 28–March 3, Ottawa. For more information, contact Integrated Computer Systems, (800) 421-8166.

User Services Wants to Hear from You

by Scott Lathrop

As our name implies, NCSA User Services is here to serve you.

We welcome and encourage your comments, criticisms, and suggestions. Notesfiles have been set up on the front-end VAX to allow you to interact with NCSA staff and other users [see the first article in this month's ***data link*** for more details]. Please use these notefiles to ask questions, pose problems, and learn from others.

Anytime you feel there are pressing problems or issues you would like to raise, you should feel welcome to directly contact the following managers within NCSA User Services.

Title	Manager's Name	Telephone (area code 217)	Electronic Mail BITNET and Internet
Assistant Director for User Services	Scott Lathrop	244-1099	13006@ncsavmsa 13006@ncsaa.ncsa.uiuc.edu
Consulting	Dave McWilliams	244-0640	13007@ncsavmsa 13007@ncsaa.ncsa.uiuc.edu
Documentation	Melissa Johnson	244-0645	11049@ncsavmsa 11049@ncsaa.ncsa.uiuc.edu
Applications Software	Brand Fortner	244-1347	14007@ncsavmsa 14007@ncsaa.ncsa.uiuc.edu
Training	Alan Craig	244-1988	13020@ncsavmsa 13020@ncsaa.ncsa.uiuc.edu
Scientific Media Services	Dan Brady	244-1995	14998@ncsavmsa 14998@ncsaa.ncsa.uiuc.edu
Scientific Visualization Program	Stefen Fangmeier	244-2003	14505@ncsavmsa 14505@ncsaa.ncsa.uiuc.edu

If you have questions about NCSA or problems getting your work done and you don't know whom to contact, please start at the top by calling or sending email to Scott Lathrop.

You can also send general suggestions to the VAX email address: SUGGEST@ncsavmsa. Your comments and suggestions will be passed along to the appropriate people to get you a timely response.

Please let us know if we can help you. §

Why Supercomputer Downtime Is Regularly Scheduled

by Doru Marcusiu

The NCSA CRAY X-MP/48 supercomputer is regularly scheduled to be out of service from 4:00 a.m. to 7:00 a.m weekdays and from 5:00 a.m. to 9:00 a.m. weekends. This time is used by the CRAY engineers for preventative maintenance and by the NCSA systems group for software testing and development.

The CRAY engineers use six hours each week to perform all needed hardware maintenance. This has resulted in the best hardware reliability for an X-MP mainframe in the history of Cray Research Inc.

The remaining hours are used each week by the NCSA systems group in their continuing effort to enhance performance and reliability of the CTSS operating system.

Downtime is used judiciously. When no systems testing is required, there is no downtime and jobs continue to run without interruption. As the reliability of CTSS has improved, availability of time on the CRAY system has averaged 99.6% over the last six months. Scheduled downtime for software testing has decreased to an average of eight hours per week.

As NCSA prepares for the migration from CTSS to UNICOS [see page 8], the systems group will be preparing for a smooth transition by using more of the regularly scheduled downtime to gain experience with UNICOS and test newly developed code needed to support UNICOS at NCSA. This is the only opportunity to accomplish these tasks.

The NCSA system group will use this time wisely and will make every effort to provide excellent service to NCSA computer users with as few interruptions as possible during this crucial phase of preparing for the transition to UNICOS.

Industrial Partner Installs Graphics Display System

by Larry White

Riaz Abdulla working at the Evans and Sutherland PS 390 high-powered graphics display system recently installed at NCSA by Eli Lilly and Company. Dr. Abdulla is a Lilly scientist working at NCSA.

Eli Lilly and Company, one of the NCSA Industrial Partners, have recently installed an Evans and Sutherland PS 390 high-powered graphics display system at NCSA. This system, which Lilly is making available to academic users and to researchers from other industrial partners, provides new capabilities for visualizing and understanding three-dimensional scientific data.

Although initial applications of the PS 390 will be in chemistry, we encourage NCSA users in other areas to test and evaluate the benefits of this system in their research as well. Existing applications may be brought to the center, and new applications can be developed or ported to work on the PS 390.

The installation of the PS 390 is a prime example of the joint benefits of the NCSA Industrial Program to the research activities of our corporate partners and academic users supported by the center. The center will benefit not only from results and understanding provided by this particular system, but also from learning and comparing the capabilities of this system as it makes a place for itself in the multivendor distributed environment at NCSA.

If you are interested in visiting the center and using its facilities, including the PS 390, you should contact the Visitors Program [see **NCSA Contacts**, page 23]. §

Enthusiasm breeds confidence in the NCSA Industrial Program.

Left to Right: D'Arcy Randall (Amoco); Larry White (Assistant Director, Industrial Program); Larry Ray (Kodak); Larry Smarr (Director, NCSA); Riaz Abdulla (Eli Lilly); John Stevenson (Associate Director, Industrial Program). Randall Luneack (Motorola) was not present when this photo was taken.

Remote Access via novaNET$^{\mathrm{SM}}$

by Sam Milosevich

NCSA is evaluating remote access via novaNET, a satellite-based wide-area computer network developed at UIUC.

The Computational Geometry research group at the University of Massachussetts in Amherst is cooperating with NCSA and the Computer-based Education Research Laboratory (CERL/PLATO) at UIUC to field-test the use of CERL networks to deliver a special NCSA supercomputer access service.

A Hybrid Network

CERL's novaNET was designed for such situations as computer-based education, where the data flow is much greater from the computer to the user than it is in the reverse. This is of interest to remote NCSA supercomputer users who wish to download large amounts of data to a workstation and have only minimal need for uploading data to NCSA computers.

A communications satellite channel carries 1.5 Mbps (million bits per second) of data from the novaNET satellite transmitter in Urbana, Illinois to all novaNET satellite receivers. Return data is carried on 9600 bps phone lines connecting each remote site with CERL. An existing Internet Protocol (IP) network connection to NCSA, such as NSFnet, also can be used for the return path.

Background Data Service

In order to provide for peak demands on the satellite channel, only 80 percent of the 1.5 Mbps bandwidth is allocated to the regular novaNET user traffic. The remaining 20 percent, or 0.3 Mbps, is available for background data sources (such as NCSA) when it is not needed for momentary peak network traffic surges.

A single novaNET satellite channel can serve many research groups from NCSA academic affiliate institutions, and additional satellite channels are potentially available.

With the current generation of file transfer protocols, the peak data rates to a remote site are observed to be approximately 150 Kbps (kilobits per second) in the aggregate with a single-user rate of approximately 70 Kbps, depending upon NCSA computer and network path.

Ethernet Bridge

The novaNET connection between NCSA and an affiliate institution is transparent to the user, once network components are installed and network routes are configured.

At NCSA, traffic destined for a remote novaNET site is routed over the campus network to CERL's gateway. All data on the CERL Ethernet are broadcast by novaNET. At a remote site, a novaNET Ethernet Bridge interface relays the Ethernet data to another gateway and then to the remote user's workstation.

The logical connection is via the standard Internet Protocol, although the bridge-class interface is protocol-independent and passes IP, DECnet, or other protocols on Ethernet. §

Email Address for Networking Questions

by Charlie Catlett

If you have problems accessing NCSA (whether via dialup, GTE Telenet, NSFnet, ARPANET, or any other path), we urge you to use electronic mail to directly contact the Networking and Remote Access Systems group at NCSA . The group's email alias is network. You may also use this email alias for general questions about NCSAnet, NSFnet, and other networks.

Electronic mail sent to this address is generally answered within two or three days. You should report more urgent problems to the consulting office. Many users are seeing a marked improvement in network access to NCSA as a result of the recent NSFnet upgrade [see ***access*** May–June 1988]. If you do not see any improvement, or if you have problems with network access, please contact the Networking and Remote Access Systems group.

The NCSA networking group is extremely concerned about any access problems you might have and would like to work with you to resolve problems. If you experience problems accessing NCSA, please send network questions, concerns, and complaints to one of the following electronic addresses:

network	(when logged into the NCSA VAX)
network@ncsavmsa	(BITNET)
network@ncsaa.ncsa.uiuc.edu	(Internet—NSFnet, ARPANET)

These email addresses will appear in **NCSA Contacts** of all upcoming issues of ***access***.

CAYLEY on CRAY Supercomputers

by George Havas

Visiting applications scientist George Havas.

I am Dr. George Havas, a professor of computer science at the University of Queensland in Brisbane, Australia. From July 1988 to January 1989 I am a visiting applications scientist at NCSA. My primary aim during this stay is to port the abstract algebraic package CAYLEY to CRAY supercomputers under UNICOS.

What Is CAYLEY?

CAYLEY is the world's preeminent package for computational group theory. It was developed at the University of Sydney (Australia), where Dr. John Cannon of the Department of Pure Mathematics and Dr. Greg Butler of the Department of Computer Science lead the development team. Currently there are over 100 CAYLEY sites in more than 20 countries.

The NCSA version of CAYLEY will be the first production version for a supercomputer.

A system for discrete algebra and combinatorial theory, CAYLEY is designed to solve problems in algebra, number theory, and combinatorial theory. Finite and infinite groups, fields, matrix rings, polynomial rings, modules, associative algebras, finite geometries, finite graphs, and linear codes are some of the structures that CAYLEY can manipulate.

CAYLEY enables users to do the following:

- perform arithmetic efficiently in groups, rings, and fields
- compute deep structural properties of groups and number fields
- study algebraic and combinatorial structures under group actions

***CAYLEY** continued on page 24*

Help Files and Online Updates

by Will Ridenour

The following online help files and documents have recently been added or updated on NCSA computer systems.

Help Files

On the CRAY X-MP/48

Batch	How to use batch files under CTSS
Charging	How NCSA charges for supercomputing time
Mathinfo	Information on mathematics software and libraries at NCSA
Memory	Information on running large memory jobs
Migration	Information on our upcoming migration to UNICOS
Nastran	How to use MSC/NASTRAN to solve a wide variety of engineering problems
Overhead	What you can do to help reduce CTSS system overhead

On the VAX Front-ends

Migration	Information on our upcoming migration to UNICOS
Training	Information on NCSA training programs for users

Documents on the CRAY X-MP/48 System

Batch	Full documentation on batch procedures under CTSS
Catalog	Online version of The NCSA *Technical Resources Catalog*

Accessing Help Files and Online Documents

To access help files on either the CRAY X-MP/48 system or the VAX front-ends enter: `help helpfilename`

To access documents on the CRAY X-MP/48 system enter: `document view documentname`

Applications Software on the CRAY Systems at NCSA

by Margaret Kubaitis

NCSA is always looking for new and more optimal software to meet the requirements of our users. Contact the software coordinator for your research area to discuss your applications software needs. The coordinators will help you if you wish to make a formal request for CRAY X-MP or CRAY-2 applications software.

Area of Concentration	**Coordinator**	**Telephone**
Astronomical Image Processing	Radha Nandkumar	(217) 244-0650
Benchmarking	Beth Richardson	(217) 333-6276
Chemistry	Harrell Sellers	(217) 333-2754
Electrical Engineering	Mark Straka	(217) 244-1991
Engineering (finite element analysis, nuclear engineering)	Ilhan Dilber	(217) 244-1973
Graphics	Mike Krogh	(217) 333-0166
Mathematics	Beth Richardson	(217) 333-6276
Parallel Methods	Michael Welge	(217) 244-1999
Symbolic Manipulation	Steve Christensen	(217) 244-0544
System Utilities	Doru Marcusiu	(217) 244-1334
Workstations	Joseph Hardin	(217) 244-6095

Software on the CRAY X-MP/48 System Running CTSS

The software listed below is currently available on the CRAY X-MP/48 system running CTSS. NCSA plans to make this software available on at least one of the CRAY systems running UNICOS. Note the column headed CRAY-2. This column indicates which applications and libraries we plan to make available on the CRAY-2 system. This list will change as we receive more information from the vendors. Given the tentative nature of this list, dates are not given for CRAY-2 availability of these packages.

The transition of software on the CRAY X-MP system running UNICOS is tentatively scheduled for the first quarter of 1989. We are depending on vendors to deliver promised UNICOS versions. We will inform users online if there is a delay in making an existing X-MP CTSS application available under UNICOS.

Changes since the last published applications software list [see ***access*** March–April 1988] include the removal of FITPACK, DYNA2D, HARWELL, and REDUCE, and the postponed installation of PASCAL and ECMFFT until UNICOS is available on the X-MP system. Installation of the CFTMATH library may be delayed on the CRAY-2 system. However, the SLATEC library, which is 95 percent of CFTMATH, will be available on both machines.

Package	**Version**	**Description**	**CRAY-2 Availability**
CFD			
FIDAP	4.1	fluid computational dynamics	y
Chemistry			
AMBER	3.0	macromolecular modeling	y
AMPAC	1.0	semiempirical molecular orbital analysis	y
CADPAC	4.0	ab initio molecular orbital analysis	y
		energy derivatives—MP2-4 correlation	y
GAMESS	1.02	ab initio molecular orbital analysis	y
GAUSSIAN86	Rev.C	ab initio molecular orbital analysis	y
HONDO	6.6	ab initio molecular orbital, GRB, CI	y
MM2	(2)	molecular modeling	y
MOPAC	4.1	semiempirical molecular orbital analysis	y
Electrical Engineering			
HSPICE	rev 5-28-87	electronic circuit simulation	y
SPICE	2G.2.5	electronic circuit simulation	y
UM-SPICE		circuit simulation	y
Graphics			

Package	Version	Description	CRAY-2 Availability
MOVIE.BYU	6.1	3D graphics/modeling library	y
NCAR Graphics	1.0	graphics package	n
PVI Contouring	4	graphics library for drawing contours	y
PVI DI-3000	5	2D and 3D (limited) vector graphics library	y
PVI GK2000	2	GKS graphics library	y
PVI Grafmaker	4	graph making package (plots)	y
PVI Metafile system	5	graphics metafile system	y
PVI TEXTPRO	2	font package	y
Mathematics			
ACM Algorithms		general math	y
BCSLIB	9	general math	n
CALMATH		CRAY X-MP assembly language math	n
CFTMATH	2.0	general math	y
ELLPACK		elliptic boundary value	y
FFTLIB	1984	NCAR FFT routines	y
IMSL	edition 9.2	general math	y
MINPACK	1	nonlinear systems solver	y
NAGLIB	MARK11	general math	y
ODEPACK		ordinary differential equations	y
PCGPAK	1.0	sparse matrix solver, iterative	y
PORT	3	general math	n
SCILIB		vector and matrix operations, FFTs	y
SMPAK	1	sparse matrix solver, direct	y
SSDLIN	1984	out of core linear systems solver	n
TOEPLITZ	none	Toeplitz form matrix equation solver	y
VECPACK	1	vector and matrix operations, FFTs	n
XMP	rev 2/86	linear programming	y
Solid Mechanics and General Engineering			
MSC/NASTRAN	65	structural analysis	n
Systems and Utilities			
BENCHLIB		general utilities, performance monitors	n
CAL	3.1	CRI assembly language compiler	y
CFT	1.14	CRI FORTRAN compiler	n
CFT77	2.0	CRI FORTRAN 77 compiler	y
HCC	2.1	vectorizing C compiler from LLNL	n

Proposed Additional Software for the CRAY X-MP and CRAY-2 Systems

The software listed below is currently proposed. The list includes planned installation dates on the X-MP system under CTSS as well as CRAY-2 availability. Installation dates are best guesses because many timelines are based on licensing and vendor delivery.

Package	Version	Description	X-MP/ CTSS	CRAY-2 Availability
CFD				
SALE3D		3D computational fluid dynamics	*	y
Chemistry				
CHARMM		macromolecular modeling	9/15/88	n
GRADSCF		ab initio molecular orbital analysis	*	n
GROMOS	(87)	molecular modeling	*	y
Electrical Engineering				
PISCES	IIB	electrical device simulation	10/31/88	y
Graphics				
NCAR (GKS)	2.0	GKS-based version of NCAR software	9/30/88	y

Package	Version	Description	X-MP/ CTSS	CRAY-2 Availability
Mathematics				
ECMFFT		fast fourier transform	*	n
EDA		exploratory data analysis	*	n
MINOS	5.0	optimization system	*	n
SLATEC	3.1	general math library	10/31/88	y
Solid Mechanics and General Engineering				
ABAQUS		finite element analysis	*	y
MAZE		2D mesh generator	9/30/88	y
NIKE2D		structural analysis	9/30/88	y
NIKE3D		structural analysis	1/31/89	y
ORION		2D plotting/post processing	9/30/88	y
TOPAZ2D		thermal analysis	9/30/88	y
TOPAZ3D		thermal analysis	1/31/89	y
Statistics				
SPSS	x2.1	statistics package	*	n
Systems & Utilities				
ANSI C		CRI C compiler	*	y
Cray Portable C	3.1	CRI C compiler	*	y
Pascal	3.3	CRI Pascal compiler	*	y

* This application will not be available for installation on the CRAY X-MP system until after NCSA converts to UNICOS production. It will not be available under CTSS.

Creating a State-of-the-art Collection of Finite Element Codes

by Ilhan Dilber

The recently formed Solid Mechanics and General Engineering Project Group. Left to right: Ilhan Dilber (user consultant), Ramesh Jayaraman (user consultant), and Mark Johnson (applications programmer). Not present when this photo was taken were Jim Kelly (applications programmer) and Jonathan A. Dantzig (UIUC associate professor of mechanical engineering).

The Solid Mechanics and General Engineering Project Group recently was formed at NCSA. The purpose of this group is to enrich the NCSA applications software collection with engineering software, particularly with state-of-the-art finite element (FE) codes as well as various pre- and postprocessing programs to supplement them.

Acquiring Software

For over a year NCSA has been trying to acquire several commercial software packages. However, the lack of vendor support for the CTSS operating system has hampered this effort to provide a good library of finite element codes in a timely fashion.

Now that NCSA is moving to the UNICOS operating system [see page 8], we anticipate that more software will be readily available from vendors. Already we have ordered some applications for the UNICOS environment for both the CRAY X-MP and CRAY-2 supercomputers, for the Alliant FX/8 minisupercomputer, and for some workstations at the IRC.

Ordering a software package is a lengthy procedure. First, the purchase must be approved by legal departments of both the university and the vendor. Then a purchase order must be issued before the vendor can prepare the tape and send it to us. Installation requires running several test programs, generally provided by the vendor, and verifying the results. The software is then tested on real-life problems. If the results are satisfactory, printed documentation (if not provided by the vendor) and, sometimes, online help are prepared. Finally, the software is released for general public use.

Existing and Planned FE Software

Recently NCSA released MSC/NASTRAN. The only other commercially supported finite element analysis code that will be installed on the CTSS operating system is MARC, which has been ordered already.

The ABAQUS tape has been received for the Alliant FX/8 computer, and a UNICOS version for the CRAY X-MP computer has been ordered. Swanson Analysis Systems Inc. (SASI) has been contacted about ANSYS for the Alliant computer and a UNICOS version for both CRAY computers.

NCSA has also been preparing to acquire additional pre- and post-processing programs. PATRAN is already available on Sun Workstations at NCSA and will be installed on both the CRAY X-MP/48 and CRAY-2 supercomputers running UNICOS. We are negotiating with Computer Aided Design Software Inc. (CADSI) for their Dynamic Analysis and Design System (DADS), which is available for the Alliant FX/8 and the CRAY-2 supercomputer running UNICOS.

In addition to the commercial software, NCSA has received several codes from Lawrence Livermore National Laboratory. NIKE2D, TOPAZ2D, MAZE, and ORION are ready for the CRAY X-MP computer running CTSS. We plan to port these codes to both computers when they are running UNICOS.

An Environment for Finite Element Analysis

NCSA is beginning to provide a rich and powerful environment for finite element analysis. If you have any suggestions, comments, or questions concerning any related software, please contact Ilhan Dilber by telephoning (217) 244-1973, or by sending electronic mail to 13024@ncsavmsa (BITNET) or to 13024@ncsaa.ncsa.uiuc.edu (Internet). §

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CAYLEY continued from page 19

Who Is George Havas?

I have been a substantial contibutor to CAYLEY, providing implementations for a number of the fundamental algorithms of combinatorial group theory including coset enumeration, subgroup presentation, nilpotent quotient calculation, and abelian group recognition.

My computing background is diverse. In addition to computational algebra, I have worked in other software technology areas, such as productivity tools for IBM-compatible mainframe environments and local area networking. In Australia I have worked on a Cyber 205 at Csironet and on a Fujitsu VP100 at the Australian National University in Canberra.

During my stay at NCSA, I will train local users and consultants to utilize CAYLEY effectively. I will also give a number of seminars, including one on the Australian supercomputing scene.

Until January 1989 you can contact me at NCSA by telephoning (217) 244-2193 or by sending electronic mail to ghavas@ncsa.uiuc.edu (Internet) or to 12372@ncsavmsa (BITNET). §

data link Preview

Conferencing by Computer—What,Why, When, and How

modified for NCSA by Alan Craig

To encourage good communication between NCSA and its users, a series of online conferences has been set up using the Notes program on the VAX front-ends. This article shows you how to access and participate in those conferences.

FIDAP 4.1 Now Available at NCSA

by Ramesh Jayaraman

There are several new features in version 4.1 of this fluid dynamics software package.

IMSL Edition 10 Available

by Beth Richardson

An enhanced and updated version of the International Mathematical and Statistical Library is now available on the CRAY X-MP/48 system at NCSA.

New Packages Enhance SPICE Capabilities for Circuit Simulation

by Mark Straka

UM-SPICE and HSPICE offer several improvements and additional capabilities over Berkeley SPICE 2G.5 for modeling problems in integrated circuit design.

Reducing System Overhead on CTSS

by Dave McWilliams

This article explains ways to reduce the CPU time used by your programs and help reduce system overhead.

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access
the NCSA newsletter
November–December 1988 vol. 2 no. 6

Science

Chaos research generates interest

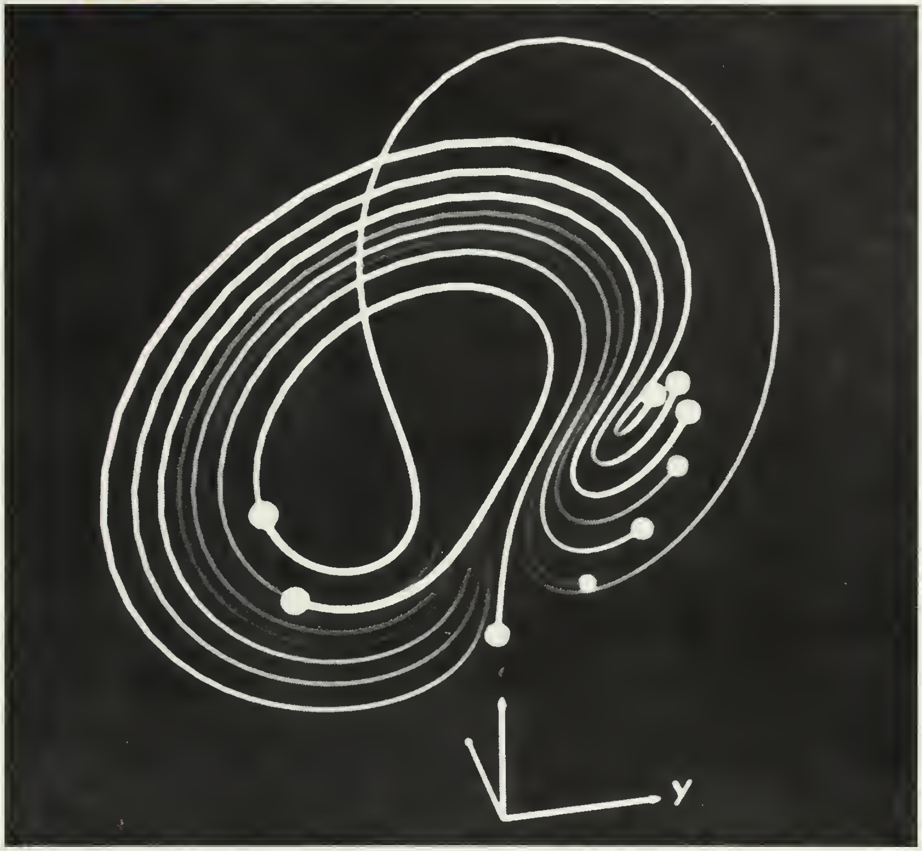
by Kathleen Robinson
Science Writer

Each of us has been convinced at least once that life is chaos. But researchers who study the confused unorganized state of primordial matter before distinct forms existed have a more cosmic view of chaos. Two NCSA staff—Michael Welge and David Hobill—have been studying chaos.

Michael Welge, a numerical consultant, heads the center's parallel processing program while pursuing his own research interests in mathematics. David Hobill is a physicist working on problems of numerical, theoretical, and astrophysical relativity. Earlier this year these two NCSA researchers combined their talents to undertake a visualization project which was immediately gratifying while leading in some unexpected directions.

They wanted to use the high-level graphics capabilities at NCSA to visualize certain well-known nonlinear systems that are the basis of the developing interdisciplinary science called chaos. Much of the work on nonlinear systems has been carried out by researchers using calculators and personal computers; flexible interaction and immediate access have been more essential to these studies than the speed or power of a supercomputer. Nonlinear dynamical systems evolve with time and can be highly sensitive to changes in initial conditions. Solutions to such systems must be obtained through numerical methods, so it seemed logical to apply state-of-the-art visualization techniques to them.

Chaos *continued on page 3*



Above. The Lorenz system can exhibit extreme sensitivity upon initial conditions. Here small perturbations in the initial conditions result in trajectories that diverge exponentially in time. Although all trajectories remain on the strange attractor, the lack of stability means that their future behavior is unpredictable.

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The newest NCSA *Technical Resources Catalog* will be mailed in January along with the next ***access***. In the meantime, refer to the online catalog for the latest documentation, publications, and software ordering information. Enter `document view catalog` on the CRAY X-MP/48 system running CTSS.

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Abbreviations

CRI	Cray Research Inc.
IRC	Interdisciplinary Research Center of NCSA
NCSA	National Center for Supercomputing Applications
UIC	University of Illinois at Chicago
UIUC	University of Illinois at Urbana-Champaign

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Left. David Hobill

Below. Michael Welge

Chaos continued from page 1

Lorenz attractor

Chaos studies have relied heavily on computers and graphics output since the 1960s, when mathematician Edward Lorenz began simulating ever-varying, short-term weather patterns. Three ordinary differential equations make up the Lorenz system. They contain just three variables and look as though they would be easy to solve. The Lorenz equations produce a stream of data that appears disorderly. Yet when the data values are plotted as points in three-dimensional space, they reveal a hidden structure. Lines connecting the points trace a double spiral in phase space that never intersects itself and never exactly repeats. This figure is known as the Lorenz attractor.

Michael Welge and David Hobill thought it would be interesting to apply the scientific visualization resources at NCSA to the Lorenz attractor. "It's a very simple system of ordinary differential equations," says mathematician Welge, "but obtaining an accurate solution through the predefined phase space requires a large number of iterations." When they first ran their code on the Sun Workstation it took about four hours. "A four-hour run on a Sun is a pretty hefty computation, compared to those being done on calculators and PCs," he adds. Later, on the CRAY X-MP/48 supercomputer, the code took just two seconds. Speed itself is not so important, but the practical effect is that many more data points can be calculated and a more detailed graphic image generated.

Scientific visualization steps in

Jeff Yost, NCSA scientific animator, next enters the picture. At his first meeting with the two chaos researchers, they gave him some files of coordinates. He was able to work up a static display of the Lorenz attractor on the IRIS workstation in about 10 minutes. "I was pretty pleased to have it come together so fast," he says. At this point, "David got excited because up until now all he had seen were static projected images of the attractor. He was down here [in the high-level graphics workroom of the IRC] for about half an hour, rotating the image and looking at it from all different angles."

The next step was for Jeff Yost to use Wavefront Technologies animation software to represent the results of the calculations as points in time and space. Due at a chaos conference in Aspen, the two researchers drove to Colorado while Jeff was still working on the animation. He was able to express mail a video to the Aspen conference in time to cause quite a stir. Chaos researchers at the conference were intrigued by a new detail revealed in the animation. The cause of the excitement was an initial transient period that precedes the chaotic behavior of the Lorenz attractor. Although its existence was known, no one suspected it would last as long as it does. Says Dr. Hobill, "Most of the chaos researchers were not aware of the power of a supercomputer coupled with visualization techniques and what this can mean for nonlinear systems work."

Numerical relativity and chaos

While working on the Lorenz system, Dr. Hobill began thinking about similar aspects of his numerical relativity work on the Einstein equations. "I started getting interested in the problem of whether the Einstein equations have chaotic behavior. The idea was to apply the methods we had learned with the Lorenz system, which is fairly simple, to the much more complex Einstein equations.

"Other researchers claim to have seen chaotic behavior associated with the Einstein equations, but we can only reproduce their results when we

Chaos continued on page 8

Developing quantum Monte Carlo methods

by Kathleen Robinson
Science Writer

"I suppose if these methods were developed today, they might have been called Las Vegas methods instead." While describing his work in condensed matter physics, David Ceperley, a physicist with joint appointments at NCSA and UIUC, was explaining classical Monte Carlo methods. These computational techniques were developed in the 1940s at Los Alamos National Laboratory in an attempt to predict the movements of neutrons in a nuclear reactor.

NCSA research scientist, David Ceperley.

Classical Monte Carlo

The Monte Carlo method for calculating the properties of a classical system is a statistical approach based on random numbers. Each particle in a liquid or solid is moved randomly. This generates a random walk and configurations that have the particles in their proper spatial distribution. Although the first application of Monte Carlo was with a random system, it also works well in situations where the underlying events are not random. Monte Carlo is unique in being useful whenever a problem consists of many particles involved in a cooperative behavior. A number of Monte Carlo variations have been developed for different applications.

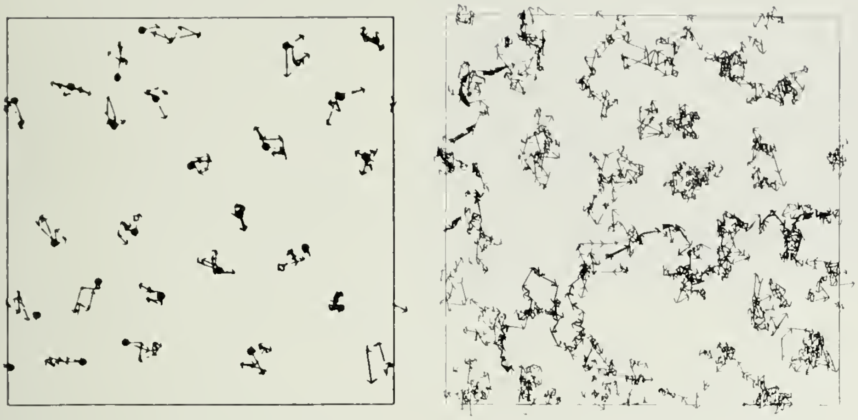
Monte Carlo and associated molecular dynamics methods have been very useful for investigating liquids and solids. More recently, protein arrangements and characteristics have been studied using classical Monte Carlo techniques. In most cases, Monte Carlo methods have been used in conjunction with the laws of classical physics.

Quantum effects

Particles at the atomic and subatomic level are governed by quantum mechanics, rather than by Newton's laws. One difference between classical and quantum physics is that in quantum physics a particle cannot both be located and have its velocity measured. This is particularly important for very light materials like hydrogen and helium. Another difference is that identical particles cannot be distinguished; an event directed at one particle may actually affect an identical particle in an entirely different region of the material. This fact has a profound effect on the behavior of quantum particles. Because classical Monte Carlo methods cannot be used to study quantum systems, Dr. Ceperley and others are developing quantum Monte Carlo methods.

Quantum clouds

One of Dr. Ceperley's projects has been to study liquid helium at the point where it becomes a superfluid—where helium atoms flow with no resistance. The figure on page 5 shows the results of a calculation on liquid helium at two different temperatures. Each atom is shown as five points—



The quantum cloud effect.

The periodic cell on the left shows a typical path configuration at $T =$ 2.5° Kelvin. Arrows connect every second point of the atom on the individual particle path. The solid dots give the various particle positions at the same instant of imaginary time.

On the right is a typical path configuration at $T = .8°$ Kelvin. The dark arrowheads indicate a path winding across the unit cell in both the x and y directions. This winding is equivalent to superfluidity, the ability to flow without dissipating energy.

the quantum cloud effect caused by the impossibility of exactly locating a particle in space. The two periodic cells shown here demonstrate that as helium is cooled, the quantum clouds become larger, forming pathways from one atom to another.

Fermion complications

Simulating helium—a boson system—is relatively simple, but the applications are limited because most particles are fermions (they have an odd number of half-integral spins). Fermions obey the Pauli exclusion principle, which says, in effect, that no two particles can occupy the same quantum state. This results in populations of particles that must be tracked separately because they are associated with regions of opposite sign. Says Dr. Ceperley, “Fermions are much harder to study but there is more motivation, because if we understood fermions then we could understand and predict the properties of all sorts of materials.”

Missing potentials

Accurate classical Monte Carlo calculations of molecular systems require a knowledge of the forces between molecules—the intermolecular potential. Unfortunately, this single essential input is not known for any except the simplest systems, and even then, often not with sufficient precision to predict characteristics such as the crystal structure. Dr. Ceperley and his colleagues are now working to calculate the intermolecular potential directly from the Schrödinger equation that describes the motions of electrons and nuclei.

Two requirements

Two requirements must be met before quantum Monte Carlo methods can be fully useful as quantitative tools. One requirement is “a lot of intellectual effort, to invent faster and more accurate algorithms,” says Dr. Ceperley. He finds NCSA’s IRC a valuable location—the interdisciplinary environment is a definite benefit. The second requirement is for more powerful computers. Again Dr. Ceperley points to an NCSA advantage. “Here we are,” he says, “on the forefront of computer technology.”

Future applications

Dr. Ceperley believes quantum Monte Carlo methods will develop into robust tools for simulating the properties of complex materials under a wide range of conditions. Other methods may be faster, but when great accuracy is needed, quantum Monte Carlo could be the method of choice. Dr. Ceperley’s plan is to use quantum Monte Carlo techniques to gauge the accuracy of the other methods, so scientists will be able to choose the tool that is most appropriate for a task.

An application of immediate interest is superconductors. “Everyone’s looking for the mechanism of superconductivity,” says Dr. Ceperley. “Why do the electrons pair up? What are their charge states? Where are the holes when you take one electron out?” The answers to questions like these may be revealed by techniques now being developed. ▲

This is the first in a series profiling research scientists on staff at NCSA.

National Academy of Sciences Symposium on Supercomputing

Role of supercomputing in industry addressed

by William Allen
Senior Science Writer

American industry has a short time in which to take advantage of the nation's lead in advanced computing technology and apply it to competitive advantage in the international marketplace, a recent symposium at the National Academy of Sciences was told.

"We have maybe a one- or two-year window to take advantage of the lead we have in supercomputing, visualization, and other advanced computing technologies," said NCSA Director Larry Smarr. "We must take them and spread them throughout the U.S. economy."

Dr. Smarr's remarks were made at the first Symposium on Supercomputing, held at the Academy in Washington, D.C. on September 9. The symposium, which brought together leading academic and corporate scientists and managers, was sponsored by the Academy Industry Program and Computer Science and Technology Board of the National Academy of Sciences, the National Academy of Engineering, and the Institute of Medicine.

The symposium—which was organized by Dr. Smarr; Doyle Knight, president of the John von Neumann Center; Steve Chen, president of Supercomputer Systems Inc.; and Professor Joseph Traub of Columbia University—explored commercial supercomputer applications as well as those emerging from university laboratories. It also outlined trends in supercomputing technology into the near future.

U.S. Senator Albert Gore, the keynote speaker, echoed the comments of several other conferees when he said he hoped the symposium was "the beginning of a new national consensus of where the United States can go" in applying advanced computing in industry, a trend that must occur quickly if American corporations are to compete effectively in the international marketplace.

Senator Gore emphasized the benefits of using supercomputers and said he was "inspired by the potential of what can happen in America" when he visited NCSA last March.

"But none of this will happen unless we solve the problems that make it an insurmountable opportunity," Senator Gore said. He urged that the government "stop chiseling away" at funding for NSF supercomputer centers. He also emphasized the need to create a national fiber optic network.

"This superhighway for information should be a number one science priority for the nation," Senator Gore said.

Dr. Smarr predicted that a new generation of students trained in supercomputing will soon enter the job market, a phenomenon that will push forward the computational science revolution in American industry. "Now, from 200 universities, you are going to have graduates coming to industry wondering where the supercomputers are," Dr. Smarr said. ▲

Eastman Kodak presentation

by Larry White
Assistant Director, Industrial Program

Dr. Clifford Perry, director of Information and Computing Technologies at Eastman Kodak Company, spoke dynamically on the benefits Kodak receives from its partnership with NCSA. He also reviewed Kodak's involvement to date and the direction they are taking with their research computing.

Among the corporate scientists and managers attending the symposium were several NCSA industrial partners as well as others who have visited NCSA, including Edward A. Mason, vice president of research for Amoco Corporation; Riaz Abdulla, manager of supercomputing applications for Eli Lilly and Company; Larry Tesler, vice president of Apple Computer; and Steve Chen, president of Supercomputer Systems Inc.

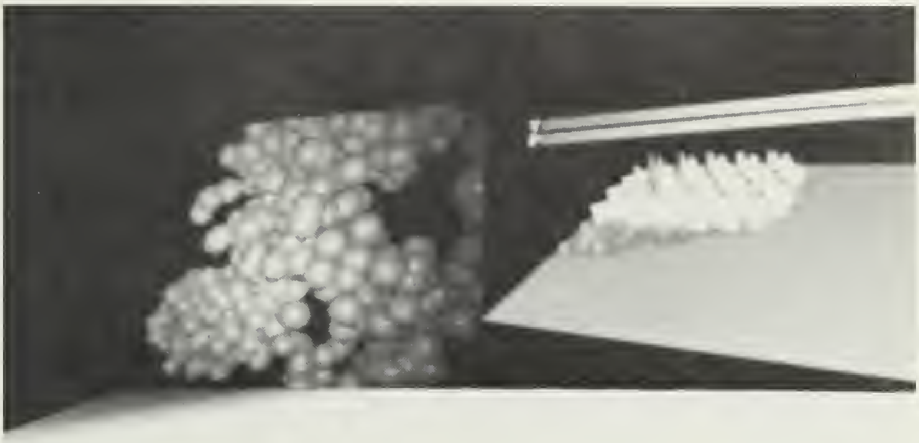
Supercomputer technology throughout the company

Kodak is working hard to spread supercomputing technology throughout the company as fast and as widely as possible. Realizing that the power of supercomputers will be on the desk of every researcher in a few years, Kodak has targeted a buy-in process whereby all corporate managers and groups of researchers identify the impact and benefits they expect from the emerging technologies of supercomputing and visualization.

Kodak's new scientific visualization video

Dr. Perry also showed a new scientific visualization videotape

A frame from the new video Kodak's Cliff Perry showed at the symposium. On the left is an image of entangled polymers and on the right is a glimpse of plastic injection molding. The video was a collaborative effort of NCSA's Carl Hoyer and Kodak's Rich Ellson and Larry Ray.



produced by Kodak at NCSA. Three Kodak projects were highlighted on this video:

- **Glyphs**
  Rich Ellson and Donna Cox
  A study of plastic flow into a mold

- **Polymer Dynamics**
  Larry Ray, Michael Rubinstein, and Carl Hoyer
  Modeling of polymer relaxation in 100 monomer chains

- **Computational Color Theory**
  Rich Ellson, Donna Cox, Jozef Cohen, Ray Idaszak, and Marc Olano
  Investigating color recognition

The videotape, set to the music of "Le Carnaval des animaux," by Camille Saint-Saens, provides a two-and-a-half minute overview of recent visualization projects done at NCSA by Kodak researchers. Carl Hoyer was the technical director for the production.

Future Kodak videotapes will be made with the help of the AT&T Pixel 932D graphics display system recently installed by Kodak in their office at NCSA [see photo below]. This system is capable of performing 500 Megaflops and can produce high-quality three-dimensional video images (images that took over four minutes to produce in the past) in just a few seconds. This system—with a 1024 x 1024 screen, dual 9-processor pipelines, and 32-pixel processors—will be used extensively by Kodak researchers to visualize their supercomputer calculations.

Kodak is meeting head on the challenge of bringing the technologies of supercomputing and scientific visualization to its scientists as a normal part of day-to-day research. ▲

Kodak's Larry Ray (left) and Rich Ellson work at the AT&T Pixel 932D graphics display system recently installed in the Kodak office at NCSA.

Help files and online updates

by Will Ridenour
Publications Editor

The following online help files and documents have recently been added or updated on NCSA computer systems:

Help files		
On the CRAY X-MP/48 system	FIDAP	Information on the FIDAP fluid mechanics package
	Batch	How to use batch files under CTSS
	CFT	Information on the CFT FORTRAN compiler
	CFT77	Information on the CFT77 FORTRAN compiler
	CFTLIB	How to use the CFTLIB FORTRAN I/O library
	IMSL10	How to access and use the IMSL10 mathematics routines
	Livermore	Information about finite element analysis codes from Livermore Labs
	Migration	Information on our migration to UNICOS
	RCFT	How to use the RCFT controller routine
	RCFT77	Information on the CFT77 version of RCFT
	SLATEC	How to use routines in the SLATEC math library
	Training	Information on NCSA training programs for users
On the VAX front-ends	Batch	How to use batch files under CTSS
	Migration	Information on our migration to UNICOS
	Training	Information on NCSA training programs for users
Documents on the CRAY X-MP/48 system	Batch	Full documentation on batch procedures under CTSS
	Catalog	An online version of NCSA's Technical Resources Catalog
	SLATEC	Information on the SLATEC general purpose math library

To access help files on either the CRAY X-MP/48 or the VAX front-ends, enter: `help helpfilename`

To access documents on the CRAY X-MP/48 under CTSS, enter: `document view documentname`

***Chaos** continued from page 3*

don't obey the constraint equations at every stage," he continued. If *all of the equations* that make up the Einstein system are not followed at every step, the solution is not correct. "Now we've gone back and solved them correctly, and it looks like we're getting some type of chaotic behavior, but it's not as dramatic as had been reported at first. We're still at a very early stage in this project."

"This is just a test"

In some respects, the animation of the Lorenz attractor was a test. "We already knew what the solution to that should look like," says Dr. Hobill, "so we could use our method and see if it came out right." Their satisfactory results gave them confidence that the method could be applied to the Einstein equations.

The impact of the test video, first seen at Aspen, continues to grow. NCSA Director, physicist Larry Smarr, generated additional interest when he showed the videotape at a meeting at the National Academy of Sciences building in Washington, D.C. A few weeks later the Lorenz attractor animation was part of the NCSA scientific visualization presentation at the 1988 SIGGRAPH meeting in Atlanta and more recently at the Supercomputing '88 Visualization Theater. The test video has been shown as part of several talks by other NCSA researchers to a variety of audiences. Soon the audience will grow significantly when an excerpt airs in January 1989 as part of a PBS "Nova" program on chaos.

David Hobill and Michael Welge are enthusiastic about the collaborative process represented by the Lorenz animation. They foresee a time when interdisciplinary work will be much more common and when graphics experts will be an essential part of any scientific team.

Says Dr. Hobill, "You always have to start with a problem. And then someone says 'I know some methods that are useful for that.' Then you need someone else who can say, 'Let's look at it from this point of view, or that point of view.' Once you start doing that, you realize how valuable and important the different sorts of expertise are."

His colleague Michael Welge gets the last word. "It's *fun* and rewarding to participate in an interdisciplinary effort." They make a convincing argument. ▲

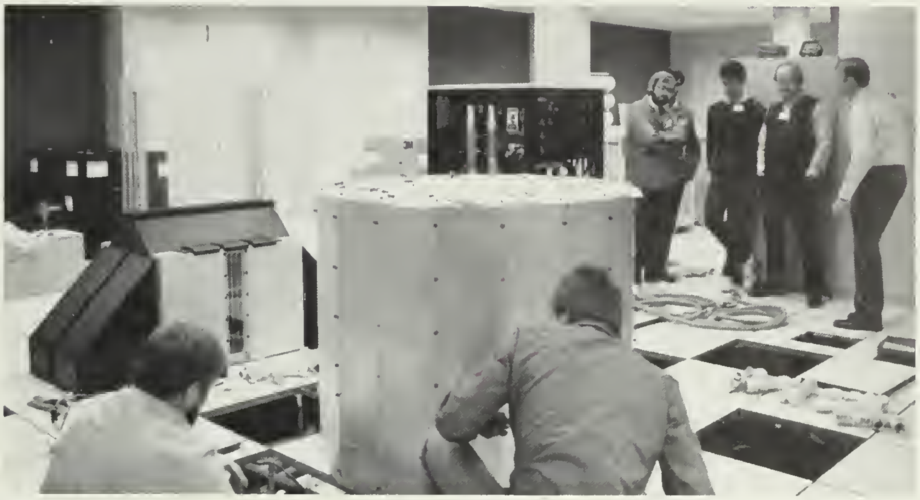
Fastest CRAY-2 system yet made installed at NCSA

by William Allen
Senior Science Writer

NCSA now has two CRAY supercomputers to meet the rapidly increasing national demand for computational power in a wide range of fields.

A CRAY-2S/4-128 supercomputer system manufactured by Cray Research Inc. (CRI) was delivered to the center on October 31. It is the first production model CRAY-2 system to feature the new and faster 45-nanosecond static-memory chips. The machine's large memory is expected to open new avenues of exploration by scientists across the nation, UIUC officials said.

The CRAY-2 system joins the CRAY X-MP/48 supercomputer currently in place at NCSA, which exists to contribute to advances in knowledge by researchers in science, engineering, economics, medicine, the humanities, and other fields. Since the center's first supercomputer arrived in October 1985, the number of researchers using the center has grown to more than 3,000 at about 150 universities and other institutions from coast to coast.



Installation of the CRAY-2 system.

Above. Dale Purdy, (Cray Research analyst in charge), Alan Carpenter and Win Bernhard (NCSA systems programmers), and Mike Smith (assistant director, NCSA systems and facilities) oversee the installation of the new CRAY-2S system.

Left. CRI technicians at work.

"The addition of the CRAY-2 system makes the University of Illinois the only university in the country with a supercomputer from both of Cray Research's lines of supercomputers," said James Bottum, NCSA deputy director. "This upgrade also increases NCSA's supercomputing power by a factor of five since the center was established."

The newly arrived machine has a 128-million-word central memory, 16 times the memory of the X-MP computer. Its peak performance speed is 1.7 billion calculations a second, about twice as many as the X-MP computer. Both machines have four processors.

The CRAY X-MP system has been used to its full capacity since last December, meaning some researchers have been unable to use the machine in a timely fashion, if at all.

"The CRAY-2 system adds much-needed capacity to a saturated NCSA," said Michael Norman, head of the center's Computational Science Program. "But more importantly, it adds new capability."

The CRAY-2's large memory will allow researchers to study problems that are both more complex and realistic, Dr. Norman said. In addition, researchers will gain a boost

CRAY-2 *continued on page 20*

UNICOS update

by Scott Lathrop
Assistant Director, User Services

The UNICOS migration plans were delayed two weeks when the delivery date of the CRAY-2 supercomputer system was changed to October 31. This change, which was announced in the September-October issue of ***access***, affected the scheduled availability of UNICOS on both the CRAY-2 and the CRAY X-MP systems. See the timeline below for the current schedule. These dates are subject to further changes based upon unforeseen developments.

December 1988	**2**	Friendly user period begins for CRAY-2S system
	5–8	First UNICOS Friendly User Training
	6	Friendly user period begins for CRAY X-MP/UNICOS system
January 1989	**9–13**	First UNICOS Training for Academic Affiliates
	23	Full production begins on the CRAY-2S system
	23–26	First UNICOS New User Training
February 1989	**1**	CRAY X-MP/UNICOS transition begins
	1	Applications due for March Peer Review Board or Small Allocations Committee
	20	UNICOS New User Training
March 1989	**6–10**	UNICOS Training for Academic Affiliates
	20–23	UNICOS New User Training
April 1989	**17–20**	UNICOS New User Training
May 1989	**1**	Applications due for June Peer Review Board or Small Allocations Committee
	4	CTSS removed from CRAY X-MP system at 4 AM
	4	Full production begins on the CRAY X-MP system running UNICOS

Updates on the UNICOS migration effort are online in the UNICOS_MIGRATION notes conference on the front-end VAX. This notesfile is also the place to post notes about problems and to get answers from NCSA staff and other users.

Please inform NCSA of any problems you encounter or any concerns you have about the migration to the UNICOS operating system. Feel welcome to contact directly the NCSA User Services managers [see **NCSA Contacts**, page 19].

If you have not yet received the updated UNICOS Migration Plan by January 10, please contact NCSA at (217) 244-0072 to receive your copy. This update will be mailed to all users in December. A *UNICOS Startup Package* will be supplied automatically to all users with UNICOS signons when full production begins in late January.

FORTRAN compilers

The FORTRAN environment will be slightly different on the two CRAY systems under UNICOS.

The CFT77 compiler will be the only FORTRAN compiler on the CRAY-2 system. Both the CFT77 and the CFT compilers will be available on the CRAY X-MP system.

If you plan to continue using the CRAY X-MP system, you do *not* need to convert to CFT77. However, reports from other centers indicate that codes compiled with CFT77 can improve performance as much as 20 to 25 percent. Also, Cray Research Inc. will be putting all major enhancements into the CFT77 compiler. Therefore, we encourage users to convert to CFT77.

Documentation

NCSA has stocked UNICOS and CRAY-2 documentation from Cray Research Inc. You may purchase these manuals at cost from NCSA. Please refer to the NCSA *Technical Resources Catalog* for ordering information—a new catalog will be mailed in January. You can also refer to the online catalog by entering `document view catalog` on the CRAY X-MP system running CTSS. If you do not have the NCSA catalog, telephone (217) 244-0072 to ask that one be sent to you. ▲

Alan Klietz, new programmer at NCSA

by Fran Bond
Technical Editor

In October, Alan E. Klietz began working at NCSA as a CRAY systems programmer. Reporting to Mike Smith and Ginger Winckler of the systems group, he is assisting with the CRAY-2 UNICOS migration program.

Prior to joining NCSA, Mr. Klietz was at the Minnesota Supercomputer Center in Minneapolis where he did CRAY-2 development work. Concurrently, he matriculated as an undergraduate at the University of Minnesota and graduated with a bachelor's in computer science with distinction in June. Eventually he hopes to pursue a master's at UIUC.

Last spring Mr. Klietz coauthored and presented a popular paper at the Cray User Group conference in Minneapolis entitled "Turbo NFS: Fast Shared Access for Cray Disk Storage."

Mr. Klietz's current interest is in compilers, particularly retargetable, vectorizing compilers. Independently he is writing a portable FORTRAN 88 compiler.

"This is a revolutionary time at NCSA," says Mr. Klietz, "and I feel lucky to be a part of NCSA right now." ▲

John Larson, new research scientist at NCSA

by Fran Bond
Technical Editor

John L. Larson, formerly of Cray Research Inc. (CRI), joined NCSA on October 26 as a research scientist working with Michael Welge in parallel processing. In addition to educating and training users in multitasking, Dr. Larson is developing algorithms and applications for the CRAY-2 and CRAY X-MP/48 systems.

As a senior applications engineer in CRI's Product Development Group, Dr. Larson supported hardware development for the CRAY X-MP multiprocessor product line. A popular speaker and author of frequently cited publications, he has conducted several CRI training sessions at NCSA.

While a senior systems analyst at Burroughs Corporation, Dr. Larson worked on the Burroughs Scientific Process and Flow Model Processor projects prior to joining CRI. A native of Champaign-Urbana, he received a Ph.D. in computer science from UIUC in 1978. ▲

First users group meeting held

Kathleen Robinson
Science Writer

Below. NSCA user and UIC academic affiliates contact Steve Roy and Patricia Wenzel, manager of NCSA user adminstration.

Sixty-four NCSA users and friends of the center met on October 17 and 18 in Urbana at the first users meeting held by one of the five national supercomputing centers. Many participants cited the pending change from CTSS to the UNICOS operating system as a prime reason for attending.

Associate Director Michael Norman launched the meeting with an overview of the impact of NCSA research. Referring to portions of the soon-to-be-published 1988 NCSA Science Report, he showed that computational science is spreading beyond its initial stronghold in the physical sciences to applied areas such as computer-aided drug design and economic modeling.

Mike Smith, assistant director–systems, reported that the NCSA CRAY X-MP/48 system is the only one in the world to run for over a full year without a hardware interruption. Showing slides of the crowded machine room and the CRAY-2 system, he posed a question which was repeated throughout the meeting. "What do the users need for a front-end on the CRAY systems running UNICOS?" About 65 percent of the users now Telnet directly to the CRAY system. Estimating that it might cost $1 million to upgrade the VAX/VMS systems, he noted that users might prefer to have that money spent in other ways. NCSA staff need to know what users want in pre- and post-processing capabilities.

Patricia Wenzel, manager of user administration, reported that there will be no changes in application procedures with the switch to UNICOS. Requests for supercomputer time have doubled and the review boards have become more selective. Explaining that many rejections result from unclear descriptions of the proposed computational methods or from inadequate justifications for the method or hours requested, she urged even renewal applicants to complete the forms carefully and to write research summaries rather than simply to attach copies of articles.

Doru Marcusiu, systems programmer, was next at the podium with an update on the current CTSS environment and the UNICOS migration plan. He encouraged more use of batch mode, saying that utilities have been modified to supply better batch status and that a fair-share job scheduler has been implemented.

The keynote speaker was Kent Koeninger of Apple Computers Inc. In his introduction, NCSA Director Larry Smarr commented that Apple may be the only corporation that thinks of a CRAY system as a personal computer. Picking up on that, Mr. Koeninger said that at Apple they "even call it a PC—personal *CRAY*, that is." He predicted that supercomputers will not be widely used by the professional and scientific population until the interface is simple enough to be used by a child of two. He argued that the simplicity of the Macintosh interface—"do *this* (pointing) to *that* " —could provide a paradigm for all computer interfaces at any level. A member of the audience asked Mr. Koeninger what he sees as a fair share of computing power to devote to the user interface. His answer, modeled on biological systems, was that eventually ninety to ninety-five percent of applications may be devoted to deciding what the user wants.

After lunch, Stefen Fangmeier, scientific visualization manager, showed part of a showpiece video with segments of many NCSA visualization projects. He described how his staff takes a project from approval by the Visualization Review Board, through discussions with the researcher, then into production using Wavefront professional animation software.

Dave McWilliams, manager of the system consultants, fielded a number of questions, including the possibility of extending consultation hours (currently 8 to 5 CST) and the tenure of part-time student consultants (they typically stay for two to three years). He said work is underway on methods for following up on referrals made to other NCSA staff, to minimize instances where a user with a problem does not get timely or appropriate advice. He also explained that the consultants cannot provide programming services, but are available to help users help themselves.

Brand Fortner, manager of applications software, urged users to suggest software they need to have on the CRAY systems, for consideration by the selection committee. He was followed by Charlie Catlett, manager of networking, who briefly described two projects that may greatly improve access to supercomputers. A project funded by AT&T is for a switched digital network that would provide 56 Kb dial-up lines [see ***access*** September–October 1988]. The other project, novaNET [see ***access*** May-June 1988], provides a satellite broadcast connection to carry data from a supercomputer back to the user, with

Left. Keynote speaker Kent Koeninger of Apple Computer Inc.

Above. NCSA user Jack Corliss talks with Dan Brady, manager of SMS.

One of the people attending the meeting was Mike Jenkins of the Boeing Corporation. Mr. Jenkins had learned of NCSA just recently when hardware he ordered included a copy of NCSA Telnet for the Macintosh. Impressed with this one product and the level of understanding it demonstrated of how workstations fit with a mainframe, he said he wondered, "Who's sharp enough to develop this?" and decided to learn more about NCSA.

Mr. Jenkins came to the User's Group Meeting to find out what else was available in mainframe and workstation connections and in graphics, parallel processing, and networking. He was excited that after two days he was going back to Boeing with six or seven solutions to his problems and "all for just $85."

Even though Mike Jenkins is not a supercomputer user, he "can see the magic at NCSA" and he can easily imagine useful applications for the new technology and software being developed at the center.

a 9600 baud phone line for the user to communicate with the supercomputer.

Dan Brady, manager of Scientific Media Services (SMS) enlivened listeners with an energetic look at how his group can help researchers communicate their results. SMS produces still photographs, slides, and video for users who are prepared to do the image preparation themselves—possibly with help from NCSA consultants.

Melissa Johnson, documentation and publications manager, talked about NCSA publications and encouraged users to turn to the NCSA *Technical Resources Catalog*, which lists documentation (including some from vendors), NCSA-produced software, and NCSA training tapes which can be ordered through NCSA. Her presentation was the last formal one before the banquet.

At the banquet Ken Bishop, academic affiliate contact from the University of Kansas, spoke informally about the eight months he spent at NCSA. He also discussed his research on underground aquifers [see ***access*** March-April 1988] and showed the video that resulted from this supercomputer research.

Early Tuesday, Joseph Hardin, manager of workstation development software, excited listeners with glimpses of updates and new developments to ImageView (formerly ImageTool), CompositeView (formerly Composite Tool), PaletteView, and the upcoming FloatView. His talk was followed by a presentation from Alan Craig, manager of user training and the Academic Affiliates Program, on user training for UNICOS operations and a brief description of the Academic Affiliates Program.

Parallel working sessions followed, with the two on scientific visualization and parallel processing drawing the largest crowds. The first NCSA users group meeting ended with reports on local programs from two academic affiliates contacts, Steve Roy from the University of Illinois at Chicago and Paul Lowe from the University of California at Riverside.

Encouraged by attendance at this first User's Group meeting, Deputy Director Jim Bottum predicted that similar—and even better—meetings may be held annually. ▲

NCSA and Cray Research announce joint software initiative

by Joseph Hardin
Manager, Software Development Group

Because of their shared interest in the future of advanced scientific computing and computational science, the University of Illinois on behalf of the National Center for Supercomputing Applications (NCSA) and Cray Research Inc. (CRI) recently entered into a joint software development project.

Cray Research has pledged $750,000 and NCSA has agreed to develop software for the CRAY-2 and CRAY X-MP supercomputers and scientific workstations. The software development projects selected for this agreement are of mutual interest to Cray Research and NCSA's user community.

The first six software development projects covered by this agreement include the following:

- NCSA will work with CRI to provide facilities in NCSA Telnet that support distributed applications, such as color Tektronix (4105) support and interactive color raster graphics.

- NCSA will work on interfaces to tools, such as HyperCard, which will permit easy capture of graphics output and quick animation of time-dependent results from applications codes running on the CRAY system.

- NCSA will work on NeWS-based distributed versions of tools such as the EMACS editor. NCSA has already developed a distributed version of EMACS for the CRAY X-MP system running CTSS.

- NCSA will develop a front-end to make the dbx debugger more usable by remote users.

- NCSA will improve and expand some documentation offered by CRI, especially in respect to the UNICOS environment. In particular, work will be done to improve the information on vectorization, optimization, and multitasking.

- NCSA will port the DOCUMENT utility from CTSS to UNICOS to provide online access to manuals. DOCUMENT was originally developed by the National Magnetic Fusion Energy Computer Center (NMFECC).

If you are particularly interested in any of these projects, please contact:

Joseph Hardin (217) 244-6095
10544@ncsavmsa (BITNET)
10544@ncsaa.ncsa.uiuc.edu
(Internet)]
or Scott Lathrop (217) 244-1099
13006@ncsavmsa (BITNET)
13006@ncsaa.ncsa.uiuc.edu
(Internet).

As NCSA Associate Director Harriett Weatherford explains, "This is just another way that NCSA is trying to work with vendors to our mutual benefit." ▲

Are you interested in working at NCSA?

by Marcia Miller
Manager, NCSA Administration

NCSA continues to grow and expand, so we have frequent openings for part-time and full-time staff. We want to encourage anyone interested in working at NCSA to submit a résumé, even before positions may actually be opened. When a position is created and a formal search is begun, we will contact those of you who have submitted résumés that fulfill the requirement of the position. After you receive this notification, you may then formally apply for the particular position, in accordance with the hiring procedures of UIUC.

We continue to advertise all open positions according to UIUC regulations, but having résumés already on file helps us identify people with appropriate backgrounds who may be interested in applying for a position at NCSA. Also, we may advertise in a city or on a date that does not catch the eye of excellent people who may be interested in working at NCSA.

We also post open positions on the front-end VAX Notes under the conference named NCSA_JOBS. This allows users of our center to log on and check on open positions at their own convenience.

We would like to receive résumés from people with advanced degrees in various scientific disciplines (including engineering, chemistry, and mathematics) and with experience in any or all of the following areas:

- supercomputing experience with large-scale systems such as CRAY computers
- parallel processing
- visualization and graphics
- UNIX
- user support (consulting, training, documentation)

Send your résumé to Marcia Miller, NCSA Administration, 152 Computing Applications Building, 605 East Springfield, Champaign, IL 61820.

NCSA is an affirmative action/equal opportunity employer.

Attention: GTE Telenet users

by Charlie Catlett
Manager, Networking

The GTE Telenet access path to NCSA has been highly underused. Our Telenet connection has a capacity of eight simultaneous users, but since February we have seen at most three users at any one time. Most often there is only one user and sometimes two or three weeks go by without any Telenet users at all. Since the cost of this service is on the order of $1000 per month, we would like to discontinue it as of January 1. 1989.If our discontinuation of GTE Telenet will impact your research, please send an electronic message to us **immediately** at one of the following addresses:

network@ncsa.uiuc.edu (Internet)
network@ncsavmsa (BITNET)
network (on the VAXes)

Thanks very much.

Allocations at the September PRB meeting

by Patricia Wenzel
Manager, User Administration

The joint NCSA–PSC Peer Review Board met on September 19 at the Pittsburgh Supercomputing Center (PSC). All of the NCSA allocations approved at this meeting were put into the queue, which is currently three months long. The board reviewed 46 proposals at the meeting, 21 from PSC and 25 from NCSA.

NCSA Proposals	Number requested	25	**Service Units (SUs)**	SUs requested	8521
	Number approved	14		SUs approved	3520
	Percentage approved	56%		Percentage approved	41%

The PRB will review applications for the CRAY-2 system for the first time at its next meeting, which will be in December.

Application Deadlines	**PRB Meetings**
November 1	December
February 1	March
May 1	June
August 1	September

Time was allocated to the following researchers at the September Peer Review Board meeting:

Alvin Bayliss, Northwestern University. Numerical study of unsteady problems in combustion.

Scott Barnett, Northwestern University. Monte Carlo simulations of crystal growth.

Joan Centrella, Drexel University. Numerical relativity and cosmology.

Geoffrey Chester, Cornell University. Simulation studies of quantum systems.

Eduardo Fradkin, UIUC. Numerical study of the Hubbard model.

John Hawley, University of Virginia. A numerical approach to black hole physics.

Frederick King, University of Wisconsin at Eau Claire. Precise energy level calculations in three-electron atoms.

Erich Krammer, UIUC. Time-dependent Navier-Stokes computations of supersonic mixing flows.

Shung-Wu Lee, UIUC. Shooting and bouncing rays.

Richard McCray, University of Colorado. Supercomputer simulation of interstellar hydrodynamics.

Fulvio Melia, Northwestern University. Accretion-induced processes in neutron star systems.

Stuart A. Rice, University of Chicago. Theoretical and experimental studies of intramolecular dynaimcs and theoretical and experimental studies of monolayers on liquids.

Huseyin Sehitoglu, UIUC. Finite element analysis of fatigue crack closure.

Ronald Taam, Northwestern University. Hydrodynamical processs in binary star systems.

S. Y. Tong, University of Wisconsin at Milwaukee. Determination of surface and interface structures by local and long-range order diffraction techniques.

K. T. Yang, Notre Dame University. Flow instabilities, bifurcations, and chaos in a three-dimensional box heated from below. ▲

“Be part of the political process,” urges Sun CEO

by Stephanie Drake
Publications Editor

Left to right. NCSA Research Scientist Steve Christensen, Sun CEO Scott McNealy, NCSA Director Larry Smarr

“I’m a U.S. flagwaver,” said Scott McNealy, CEO and cofounder of Sun Microsystems Inc., in a recent talk to the UIUC Sun User Group. Since he joined the American Electronics Association (AEA) board of directors, Mr. McNealy has had an close-up view of U.S. and world politics.

What he sees leaves him concerned. The ultimate power to change anything is held by the world economic powers, and future world economic powers will be the leading technological countries. This belief left him particularly concerned about the 1988 presidential debates: both candidates demonstrated “absolute ignorance of and inattention to technology.” The upbeat side is that in this country citizens involved in politics can exert influence.

He pointed to the development of UNIX as an example of how the government can play a role in technological developments. Bill Joy was one of the prime developers of the Berkeley version of UNIX on a DoD grant. Then Berkeley got UNIX off and running because it gave the technology free to graduate students.

A role in the world economy

The CEO of Sun Microsystems enjoys a unique view of the world. Founded six-and-a-half years ago, Sun Microsystems’ revenues have gone from zero to well over one billion dollars. It is now a Fortune 250 company. Staff has grown from zero to 7500, an unprecedented rate of growth, and Sun is still hiring 200 to 250 people each month.

Introducing Mr. McNealy, NCSA Director Larry Smarr said, “What’s exciting is the change in the way scientists think about their research because of what sits on their desktops. That’s what’s really exciting about what Sun has done. . . . They’ve kept the *fun* in computers.” Scott McNealy simply says, “I’ve got the best job in the computer industry!”

Again, economic power plays a key civics role. Sun Microsystems exported $12 million worth of products in October. That kind of export adds to the U.S. tax base, helps lower the paralyzing U.S. trade deficit, and helps improve the worldwide standard of living.

“Our problem is that we think all cultures are like ours.” Mr. McNealy pointed to the serious shortage of DRAM. Computer industry growth is absolutely limited by lack of DRAM. U.S. manufacturers tell Mr. McNealy that they’re concentrating on other components because DRAMs aren’t profitable. Meanwhile, Japanese manufacturers say that to buy their DRAM companies must first purchase other components. And 85 percent of DRAM in the world is made in Japan.

McNealy on the computer industry

Scott McNealy sees “the computer industry going through massive consolidation now” and thinks it will be interesting to watch the computer industry change over the next five to ten years. He left the Sun User Group with a couple more thought-provoking tidbits: “In this industry, you don’t want to be the first to develop a concept—you want to take someone else’s concept and develop it into a better product. . . . If you’re chasing standards instead of setting standards, you’re lost. ” ▲

NCSA Academic Affiliates

As of November 30, 1988

Clemson University
Charles Heck
(803) 656-4307

Colorado State University
Patrick Barns
(303) 491-1575

Duke University
Shiangtai Tuan
(919) 684-3695

Eastern Illinois University
Dave Henard
(217) 581-3227

Gallaudet University
Donald V. Torr
(202) 651-5027

George Washington University
Thomas E. Moyer
(202) 944-6389

Georgia Institute of Technology
Mary Trauner
(404) 894-6166

Harvard University
Lewis Law
(617) 495-2627

Illinois Institute of Technology
Robert van Borstel
(312) 567-5962

Indiana University
Robert Holden
(812) 335-9258

Kansas State University
Neil Erdwien
(913) 532-6311

New Mexico State University
Joseph R. Denk
(505) 646-3439

New York University
Jeff Bary
(212) 998-3049

North Dakota State University
Mark Gordon
(701) 237-8011

Northern Illinois University
Samnuan Duramad
(815) 753-1057

Northwestern University
Albert Lunde
(312) 491-4093

Oklahoma State University
Nancy Stevens
(405) 624-6301

Oregon Graduate Center
Jon Crowhurst
(503) 690-1035

Oregon State University
R. J. Murray
(503) 754-2494

Pennsylvania State University
Molly Mahaffy
(814) 865-4750

Rose–Hulman Institute of Technology
Bruce Danner
(812) 877-1511

Southeast Missouri State University
Anthony J. Duben
(314) 651-2785

Southern Illinois University at Carbondale
Larry Hengehold
(618) 453-4361

Stanford University
Randy Melen
(415) 497-2300

State University of New York at Buffalo
Geraldine Sonnesso
(716) 636-3550

State University of New York at Stony Brook
Arie Kaufman
(516) 632-8441

Syracuse University
Wayne Fordyce
(315) 423-3998

Tufts University
Austin Napier
(617) 628-5000

University of Alaska at Anchorage
Valerie Johnston
(907) 786-4849

University of Alaska at Fairbanks
Conrad Deitz
(907) 474-6328

University of Arkansas
Bill Ashmore
(505) 575-2905

University of California at Irvine
Herbert W. Hamber
(714) 856-5596

University of California at Los Angeles
Maha Ashour-Abdalla
(213) 825-8881

University of California at Riverside
Paul N. Lowe
(714) 787-3883

University of California at Santa Barbara
Bob Sugar
(805) 961-3469

University of California at Santa Cruz
Dennie van Tassel
(408) 429-2578

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(312) 702-7575

University of Colorado
Richard Jones
(303) 492-3865

University of Delaware
Dean Nairn
(302) 451-1718

University of Idaho
Terry Leung
(208) 885-6554

University of Illinois at Chicago
Steve Roy
(312) 996-2489

University of Iowa
Judy Brown
(319) 335-5552

University of Kansas
Michael Grobe
(913) 864-4965

University of Maryland
Jack Hahn
(301) 454-5434

University of Missouri at Columbia
Lew Davison
(314) 882-2112

Training sessions for new supercomputer users

by Alan Craig
Manager, User Training

Due to the transition from CTSS to UNICOS, NCSA offered its final two-day CTSS training session in October. NCSA training now helps both migrating users and new users get started with UNICOS. The UNICOS New User Training sessions will be three-and-a-half days long. Enrollment is limited.

1989	January 9-13	UNICOS Training for Academic Affiliates
	January 23–26	UNICOS New User Training
	February 20–23	UNICOS New User Training
	March 6–10	UNICOS Training for Academic Affiliates
	March 20–23	UNICOS New User Training
	April 17–20	UNICOS New User Training

You must have a CRAY userid to register, and you must register at least one week before the session. To register for a training session or to get more information about the training program, please contact the NCSA Training Program [see NCSA Contacts, page 23]. To see the latest training schedule, enter `help training` on the VAX or CRAY computer.If you would like to extend your visit at NCSA beyond the training program dates, contact the NCSA Visitors Program [see NCSA Contacts, page 19].

University of Missouri at Kansas City
Charles Volk
(816) 276-1481

University of Missouri at Rolla
Dan Uetrecht
(314) 341-4841

University of Missouri at St. Louis
Larry Pickett
(314) 553-6000

University of Nebraska at Lincoln
Dr. Gerald Kutish
(402) 472-5220

University of Nevada at Las Vegas
James Williams
(702) 739-3557

University of New Hampshire
Elizabeth Rivet
(602) 862-1570

University of New Mexico
Art St. George
(505) 277-8036

University of Notre Dame
Milind Saraph
(219) 239-7240

University of Oregon
Patrick Holleran
(503) 686-4394

University of Rochester
Richard Phillips
(716) 275-2811

University of Tennesse at Knoxville
Sue Smith
(615) 974-6721

University of Tulsa
Albert C. Reynolds
(918) 592-6000

University of Washington
Steve Halstrom
(206) 543-9700

University of Wisconsin at Madison
Wayne Shockley
(608) 262-3724

University of Wisconsin at Milwaukee
David Stack
(414) 229-4041

Vanderbilt University
Maria Perkins
(615) 322-7311

Washington State University
Lynn Cannon
(509) 335-0412 ▲

Scientific visitors at NCSA

Charles Evans. December 4–12 from California Institute of Technology. Area of research: Astrophysics.

Philip Hardee. December 13–17 from University of Alabama at Tuscaloosa. Area of research: Astrophysics.

Paul Kilbride. December 5–9 from University of Illinois at Chicago. Area of research: Opthalmology

Chris Kochanek. December 4–12 from California Institute of Technology. Area of research: Astrophysics.

Theodorus Koupelis. December 13-17 from University of Alabama-Tuscaloosa. Area of research: Astrophyics.

NCSA Contacts

General information

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(217) 244-0072

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Documentation and Publications Orders
Kay Weidner
(217) 244-8045

CRAY Operations
(217) 244-0710

Industrial Program
(217) 244-0474

Networking
network (VAX)
network@ncsavmsa (BITNET)
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Relativity Mailing List
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14008@ncsavmsa (BITNET)
steve@ncsa.uiuc.edu (Internet)

Visitors Program
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(217) 244-0074
uadmin@ncsavmsa (BITNET)
uadmin@ncsaa.ncsa.uiuc.edu (Internet)

Machine access and information

Dialup Access—2400 baud or less
(217) 244-0662

Dialup Access—9600 baud
(217) 244-6733

VAX Telenet Address
217 35

CRAY X-MP/CTSS IP Address
ncsad.ncsa.uiuc.edu (128.174.10.48)

CRAY X-MP/UNICOS IP Address
ux.ncsa.uiuc.edu (128.174.10.46)

CRAY-2 IP Address
u2.ncsa.uiuc.edu (128.174.10.44)

Front-end VAX Mail Address
user@ncsavmsa (BITNET)
user@ncsaa.ncsa.uiuc.edu (Internet)

Front-end VAX IP Address
ncsaa.ncsa.uiuc.edu (128.174.5.100)
ncsab.ncsa.uiuc.edu (128.174.5.101)

NSFnet Problems
(617) 873-3400

NSF Network Service Center
nnsc@nnsc.nsf.net

ARPANET Problems
(800) 235-3155

SRI-Network Information Center
(415) 859-3695
nic@sri-nic.arpa

User services managers

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14505@ncsaa.ncsa.uiuc.ed (Internet)

CRAY-2 continued from page 9

from the CRAY-2's ability to perform parallel processing—splitting up problems into parts that are solved simultaneously for great speed.

Many of the studies conducted using the CRAY X-MP system have been limited to analysis in two dimensions. The CRAY-2 system opens up the potential of three-dimensional analysis and other new horizons for researchers studying thunderstorms, the chemistry of large biomolecules, earthquakes, astrophysical events, the design of computer circuits, and hundreds of other problems.

Robert Wilhelmson, UIUC professor of meteorology who leads a group at the center studying the development of severe storms, said the CRAY-2 system's large memory, parallelism, and UNIX environment will change the way he thinks about simulating these storms to unlock their inner workings.

Using another CRAY-2 system, Dr. Wilhelmson and his colleagues already have gained new information about the region within storms where tornadoes form, about the factors distinguishing storms that produce lots of rain from those that produce little, and about storms that produce tornadoes within hurricanes. The NCSA CRAY-2S system will allow new kinds of explorations.

"We will be able to do things we haven't done yet with the intent of learning more about severe storms and tornadoes," Dr. Wilhelmson said. "We will actually carry out the storm simulation when we want, continuing it, altering some of the parameters. This makes for more effective use of the supercomputer and the user's time."

The NCSA CRAY-2 system will undergo a shakedown period in November and December and will open to the national user community in January. ▲

data link Preview

Notes and Quick Tips
A new ***data link*** feature, this section offers updates, solutions to problems, and announcements for NCSA users.

Batch Classes: Accommodating different job requirements on the CRAY X-MP/48 system
by Shyam Kumar Duggirala and Ilhan Dilber
This article offers information on specifying the correct class for your batch jobs for the quickest possible turnaround time and smooth operation.

CFT and CFT77 differences
by Jim Ferguson
With NCSA's migration to UNICOS, this article offers some timely information on converting your FORTRAN codes to use with the CFT77 compiler.

SLATEC library available
by Beth Richardson
This article introduces the large general purpose math library now available on the CRAY X-MP/48 system. ▲

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Science

Discovery of new life form leads to genome analysis center

by Kathleen Robinson, Science Writer

The recently formed Center for Prokaryote Genome Analysis (CPGA) is headed by Carl Woese, an evolutionary geneticist at UIUC, and Jordan Konisky, head of the UIUC Department of Microbiology.

A 1984 recipient of the MacArthur Fellowship and recently elected to the National Academy of Science, Carl Woese is best known for having recognized that a primitive type of organism—previously grouped with the bacteria—might actually constitute a third form of life on earth.

Below. Carl Woese and Jordan Konisky, directors of the recently formed Center for Prokaryote Genome Analysis.

Two types of cells

For many centuries, life was thought to be of two basic kinds—animal or plant. In the mid-nineteenth century biologists realized that there were certain microscopic organisms—protists—that were not specifically related to either animals or plants. By the mid-1940s it became clear that the most fundamental distinction among living systems is based on whether or not a cell possesses a nucleus—whether its genes are held in a membrane sac. Cells with a well-defined nucleus (this includes both plants and animals) are *eukaryotes*. Cells without a well-defined nucleus—presumed to be a more primitive life form—are called *prokaryotes*; bacteria fit in this group.

Genetic studies

One method geneticists use to study the relationships among organisms is to compare the sequence of *nucleotides*

***Genome analysis** continued on page 3*

FMC is newest industrial partner

See story on page 10.

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Abbreviations

CRI	Cray Research Inc.
IRC	Interdisciplinary Research Center of NCSA
NCSA	National Center for Supercomputing Applications
UIC	University of Illinois at Chicago
UIUC	University of Illinois at Urbana-Champaign

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***Genome analysis** continued from page 1*

(nucleic acids) in the molecule 16S ribosomal RNA. This molecule is a component of the ribosome, the molecular machine that synthesizes proteins. (The designation 16S refers to the speed with which the molecule sediments in a centrifuge, measured in Svedberg units.) Ribosomal RNA is easy to isolate in workable quantities because a typical bacterial cell has from 10,000 to 20,000 ribosomes.

Specific enzymes are used to clip 16S ribosomal RNA into short segments (called *words*), each containing from one to twenty nucleotides (called *letters*). Words of six or more letters are compiled into a dictionary. Dictionaries of different organisms can be compared in terms of an association coefficient which reveals the degree of relatedness among the organisms. Significantly similar dictionaries indicate a common ancestor.

Word length is measured through the use of sequencing gels. Gels separate molecular fragments on the basis of mobility through the gel matrix when an electric field is applied. The number of nucleotides in each word can be determined by this method.

Archaebacteria—an old life form newly discovered

In the early 1970s, UIUC scientist Ralph Wolfe devised techniques for culturing certain methane-producing prokaryotes called *methanogens*. With Dr. Wolfe's help, Carl Woese included these hard-to-grow organisms in his study of ribosomal RNA that had begun a few years earlier. When Dr. Woese and his colleagues compared the ribosomal RNA of methanogens with that from other prokaryotes and eukaryotes, they noticed that in certain essential ways the methanogens were as different from the other prokaryotes as they were from the eukaryotes. Based on this and subsequent evidence, they proposed that the methanogens might represent an evolutionary branching that antedated the common ancestor of the other, "true" bacteria. Being anaerobic, methanogens have metabolisms that are well suited to the conditions that may have prevailed in the early years of life on this planet. Dr. Woese called this new primary kingdom *archaebacteria*.

Computationally challenging

Dr. Woese recalls that the early discoveries led to more and more questions. "It became increasingly apparent that if we really wanted to understand organisms—especially the deeper aspects of evolution—we would have to sequence not just one type of gene, but the entire complement of genes. This was something that one didn't even *think* of ten years ago because it seemed such an enormous task."

One of the people who didn't consider genome analysis impossible was NCSA Director Larry Smarr. "When it became known that Larry Smarr saw this work as computationally challenging—a future-oriented project—it began to get off the ground," recalls Dr. Woese.

Genome analysis center takes shape

CPGA represents a research initiative begun on a relatively modest scale that has grown to require a higher level of support. It received a $400,000 NSF Biological Center grant followed by a $1,150,000 (over five years) joint software development grant from Amoco Corporation. Additional funding is being sought as the CPGA takes shape. Soon to be housed partly in the Beckman Institute [see ***access***, July-August 1988], the CPGA will retain its original collaborative, interdisciplinary nature, but will gain greater national status.

CPGA has four functioning units. One unit is involved in the mapping of bacterial genomes, determining the order and spacing of "marker" genetic segments. The second CPGA unit does the actual sequencing of genomes. These two units together constitute the biological side of the research. A third unit is involved in technology development, working on a device for reading the sequencing gels. This is a computationally intense process, since the software must read the gels at well over 99 percent accuracy. The fourth, or analytical, unit will revolve about the construction of a large and sophisticated database that biologists will use to handle and interprete sequence data and then relate these to other types of biological data. Says Dr. Woese, "It is in terms of the third and particularly fourth unit that our interaction with NCSA will be very important."

Research agenda

According to Dr. Woese, "This work is, in one sense, a necessary warmup for the bigger task of sequencing the human genome." As an evolutionist, he is not particularly interested in the human genome, although he acknowledges that from a medical perspective it is important. "In the realm of evolutionary studies," says Dr. Woese, "we want to be able to define the small number of aboriginal cell families from which all the genes in a eukaryotic cell have presumably evolved. In more of a molecular realm, we hope to be able to understand the structure of genomes, and we want to be able to contribute to studies of the three-dimensional structure of proteins and nucleic acids—we will be interacting with researchers interested in molecular structure."

Education agenda

As a professor of microbiology, Dr. Woese has an additional, pedagogical goal. "We also want this project to serve as an impetus for generating a computer biology curriculum that will create biologists who genuinely understand computers—not just to be able to use computers, but to understand their potential for structuring research and opening new directions."

With a modesty that is by all reports characteristic, Dr. Woese downplays his role in the events that led to the formation of the CPGA. "It's not that my insight was all that great," he says, "it's that technology changed at a certain point in time so that one could do these things. I happened to be the first to realize that it was important to do this [sequence analysis] for bacteria."

Be that as it may, many people feel the world could use more scientists with the insight of Dr. Carl Woese. ▲

Ongoing opacity project is an international effort

by Dimitri Mihalas, NCSA Research Consultant, UIUC Professor of Astronomy,and Member, National Academy of Sciences

Seventeen scientists from the United Kingdom, France, West Germany, Venezuela, and the United States are working on a long-term project to compute radiative opacities for stellar envelopes. Their most recent meeting was held December 19–21 under NCSA auspices at the Beckman Institute for Science and Technology and was the first scientific meeting conducted by the center at the newly opened Beckman Institute.

This group of scientists consider opacity a critical physical parameter because it determines the rate at which radiative energy can be transported through a star. This means that opacity very sensitively affects how a star evolves and how it can pulsate. A stellar envelope includes all layers of a star outside the dense core, where thermonuclear reactions release the energy radiated by the star.

Until recently, astrophysicists were almost totally dependent upon Los Alamos National Laboratory to provide the opacity data they needed to study stars. But the availability of supercomputers in national centers in the United States now makes it feasible for university scientists to carry out these complicated calculations. For the first time it is possible for the scientists who actually use the numbers to generate the particular data they need.

The opacity project

The Opacity Group's project consists of three parts that are separate but interrelated:

- generating atomic photoionization cross sections and spectrum line strengths
- calculating an equation of state describing the distribution of atoms among various excitation states and ionization stages
- combining both datasets to produce both detailed spectral information about the absorptivity of stellar material and mean values appropriately averaged over the spectrum.

The atomic data are being computed primarily by two large groups centered in London and Belfast, led by Professors M. J. Seaton and P. G.

Physicists honor Larry Smarr

by William H. Allen, Senior Science Writer

NCSA Director Larry Smarr has been elected a fellow of the American Physical Society, the highest level of membership in the nation's leading society of physicists.

Dr. Smarr, who is also a professor of physics and of astronomy at UIUC, was cited by the society as a "pioneer in the field of numerical relativity, expert on relativistic hydrodynamics and its application to realistic astrophysical scenarios, and farsighted organizer of a national supercomputing center for the benefit of all sciences."

About 10 percent of the society's 40,000 members are fellows. ▲

Above. NCSA Director Larry Smarr.

Left. Addressing his fellow researchers at the opacity workshop, Professor Michael J. Seaton (University College, London) describes his recent work on line broadening of hydrogenic ions.

Burke respectively, with support from isolated investigators in the other countries represented at the meeting. These two groups have the world's most advanced codes for computating atomic structure and the radiative properties of atoms. The higher quality data being generated with these codes offer the opportunity for substantial improvements over earlier work.

The equation of state has been developed by members of the United States team and resides at NCSA. This computation is based on a free-energy minimization for some 200 independent species in the plasma for various choices of representative stellar compositions. The method uses an *occupation probability* formulation which describes how high-lying states are destroyed by interactions with charged particles in the plasma. Data from these computations have already been released to the astrophysical community.

The final stage of the calculation, the opacity code, is also being developed at NCSA. The code has been designed to function effectively on both the CRAY X-MP and CRAY-2 computer systems at the center. Care has been taken to resolve adequately all sharp features in the spectrum: spectrum lines and continuum resonances. The final calculations will use an immense database of 200 to 300 Megawords—all of which must be online during the calculation of tables covering a wide range of temperatures and densities. This huge calculation will make heavy demands on both machines at NCSA. It is currently estimated that early results from the full calculation will begin to become available in early 1990.

While visiting UIUC . . .

During their stay in Urbana-Champaign, the members of the Opacity Group also visited the Center for Supercomputing Research and Development (CSRD) to learn about the approach to parallel processing taken by the Cedar Project under the direction of Dr. David Kuck. They also toured NCSA facilities to see firsthand some of the equipment they had previously known only via remote networks. ▲

In the Opacity Group

United Kingdom

K. A. Berrington
P. G. Burke
V. M. Burke
W. Eissner
A. Hibbert
A. E. Kingston
H. E. Saraph
M. J. Seaton
P. J. Storey
K. T. Taylor

United States

D. G. Hummer
D. Mihalas
A. Pradhan
Yu Yan

France

C. Zeippen

West Germany

K. Butler

Venezuela

C. Mendoza

Making the future happen today

by Kathleen Robinson, Science Writer

As an NCSA research scientist, Steve Christensen has a multidimensional role. A physicist active in quantum gravity theory, Dr. Christensen is also an expert in high-performance workstations and the software used on them. At NCSA, he is behind the symbolic computing software development effort. He is president of the newly formed national *Mathematica* Users Group, and is on the Board of Directors of the international Sun Users Group. Dr. Christensen works closely with the companies that design workstations. His personal goal is to push workstations to higher and higher levels of performance.

Workstation power

One of Dr. Christensen's jobs has been to compare what present supercomputers do well with what is done best by desktop workstations instead. "Supercomputers are designed to do floating point calculations very well, but they are not especially useful for the type of physics I do, where the non-floating point calculations get enormous. In symbolic computing, we build equations with—literally—millions of terms." He and his colleagues don't often need the number crunching capabilities of a supercomputer because their equations consist of many symbols rather than numbers. Their goal is to reduce the millions of terms down to a few dozen or so. "We're inventing programs to do these calculations on high-performance workstations, which tend to be faster at this kind of work than current supercomputers. Ultimately, it is the combination of machines that is important—not just the supercomputer and not just the workstation, but the two together."

Below. Dr. Christensen is shown working at his NeXT computer. This machine—which has 8 megabytes of memory, a 330 megabyte disk, and 246 megabyte optical disk—was the first NeXT development machine on the UIUC campus and one of the first delivered in the nation. Given its interesting shape and color, Dr. Christensen has dubbed it Darth Vader.

Tensor algebra project

While pursuing his research in quantum gravity theory, Dr. Christensen is working on the symbolic computing software tools necessary for that research. He and a colleague from the University of Wisconsin, Leonard Parker, are developing a package to do tensor algebra using the program *Mathematica*. They expect to have a version ready by next summer. Says Dr. Christensen, "I think anyone who does tensor manipulations will probably want it, partly because it's very changeable. It's not code in the usual sense—it's not something you compile. It's a bit like an expert system—a database and rules for how to get from point A to point B in the calculation. There are other tensor systems, but they are not as modern, not as powerful, I think."

Thousands and millions

Dr. Christensen has been able to generate equations with millions of terms using current software and equipment, but the existing tools take a long time to simplify such large equations. The equation he is currently working with—which contains "only sixteen thousand terms"—took two hours to generate on the Sun-4, and forty-six hours of continuous Sun-4 running to analyze. Given such statistics, it is easy to see how higher performance is necessary before equations involving millions of terms can be manipulated.

No room for error

One might expect some latitude for error in calculations involving thousands and millions of terms, but this is not the case. “If the calculation is not done perfectly, the answer we get will be utterly wrong. We are dealing with concepts like the structure of the universe. One little mistake in the million terms—a plus sign, a minus sign, a factor of two—can change our notion of whether the universe will expand forever, or whether it will collapse.” To check for computational errors, the programs must be able to run the calculations in several ways and compare the answers.

Anticipation

Besides the usual academic clutter of books and journals, crowded into Dr. Christensen’s office are five workstations, including a recently delivered NeXT system. As a researcher who is pushing these machines to their limits, Dr. Christensen has a strong personal vision of improvements he would like to see in workstation technology.

He launches into his list without hesitation—almost without pausing for breath. “Calculations that take me forty-six hours—to be able to do them in one hour. A very, very interactive computer screen. I want to point to an equation with a mouse, and do something with a term exactly as I used to with paper and pencil. I want to pick up a term and physically move it to another place. Equations on the screen should look like they are printed in a book or journal, and not like computerese. Tools should permit me to tell the equation to do things. The computer should be like a colleague, like a blackboard, like ten graduate students. Instead of giving ten graduate students my equation to do and having them make a hundred mistakes and work it and work it and work it, have the computer do it, perfectly. And furthermore, be able to link this computer screen with my colleague’s screen in Texas and have him be able to see the same thing I’m seeing, so we’re both working interactively on the same equation on the same machine. Have all the journals online, so that if my colleague remembers a reference, we can bring up that paper on the screen and look at it together. I want to have intelligent programs that can tell when some especially heavy calculation needs to be done, then ship the work off to a supercomputer, perhaps, somewhere on the network—automatically—without me having to request it.”

Above. A Sun-4/260 computer with 64 megabytes of memory, 881 megabytes of disk, a high resolution monochrome monitor, and a color monitor is Dr. Christensen's current large-scale symbolic manipulation research machine. The machine's name is Yoda. Also shown are a Sun-3/160 and a Macintosh II.

Coming soon . . .

“I don’t think this is just vision,” he insists, “I think it will be reality in the near future. Many of the pieces are already here. The ability to write equations on the screen nicely will certainly exist very soon—people are working on it now. Faster machines are just around the corner. In two years’ time I’ll have a machine smaller than my Sun that’s ten times faster. The business of linking together five or ten machines all working on the same problem at the same time—I know it can be done, I just haven’t figured out the code that does it. I feel lucky that I’m young enough so I’ll have twenty or twenty-five years to play with this technology.”

“What’s going to happen is that the software to do symbolic manipulation will become a general scientific tool—it will affect the numeric people. They will do a lot with their basic equations before trying numbers with them. We all will use the supercomputer less, but much more effectively—which is good. There aren’t that many supercomputers—they’re expensive machines. So the more we can use them to do just what they’re best at, the better off everybody is.” ▲

Creating tools for science

by Joseph Hardin, Manager, Software Development Group
Ann Stowell, Support Staff, Software Development Group
Fran Bond, Technical Editor

If, like thousands of people across the country, you start your workday on an IBM PC, Macintosh, or Sun Workstation by signing on to a com-puter across the NSFnet or a local machine across a TCP/IP network, there is a good chance that you are familiar with at least one of the products of the NCSA Software Development Group (SDG)—NCSA Telnet. Like hundreds of researchers, you may also use NCSA Image to observe on your own workstation color images of the simulations you have run on a large compute engine like a CRAY system.

These programs demonstrate SDG's purpose: to develop tools that allow computational scientists to efficiently and productively use the supercomputer resources now available. Frequently this purpose demands the development of software for the workstations that sit on researchers' desks, not for the supercomputers. The SDG staff believe that the workstation—often a relatively powerful system in its own right—is the researcher's window into the workings of a supercomputer. The researcher's workstation often has capabilities that can enhance and facilitate scientific study and analysis, if integrated into research done with the aid of the supercomputer.

Visualization tools

Researchers have discovered that visualizing the results of computations on machines such as NCSA's CRAY X-MP and CRAY-2 systems is as important as the ability to compute large problems. The enormous mass of numerical data generated by a supercomputer necessitates a way to interpret results and gauge the success of supercomputer simulations. But tools for scientific visualization of computational results have often lagged behind the development of powerful compute engines. Initially, visualization techniques were available to only a small group of users with access to specialized hardware or software resources. But for the current revolution in computational science to have the greatest possible impact, such capabilities must be put in the hands and on the desks of the average user.

Responding to researchers' needs for refined software tools with which to depict, observe, and interpret the intricate processes and computations done on supercomputers, SDG develops programs that allow scientists to construct images from data, and thereby observe the patterns and novel or unexpected behaviors of the phenomena under investigation. SDG strives to bring to the computational science community as near state-of-the-art capabilities as the currently installed base of user hardware will support —and as quickly and cost effectively for users as possible. Visualization tools developed by SDG are generally useful not only to supercomputer users, but also to anyone trying to extract information from large datasets, including satellite, sonic, and medical imaging data.

SDG develops concepts for software tools, converts them into releasable products, and transforms prototypes offered by scientific researchers into unique, instrumental, and serviceable software packages that are suitable for various workstations. SDG concentrates on producing effective workstation software that encourages and enhances communications, data analysis, and visualization. All of SDG's software, documentation, and source codes are released into the public domain to maximize their availability to users and their potential for extension by other developers. It is also available through the NCSA *Technical Resources Catalog*. [The January 1989 issue of the catalog accompanies this newsletter.]

Recent releases

A wave of recent activity by SDG has placed several important tools in the hands of scientific researchers. The SDG team recently has released the software described in the following paragraphs.

NCSA Telnet Version 2.2

Tim Krauskopf, SDG's design leader, and Gaige Paulsen, programmer, developed NCSA Telnet Version 2.2 for the Macintosh and the PC. An implementation of DARPA standard telnet with additional features, NCSA Telnet is a popular means of providing interactive access from a Macintosh or an IBM PC and compatibles to telnet hosts on TCP/IP networks. Senior Programmer Martin Knapp-Cordes and Programmers Heeren Pathak and Quincey Koziol have joined the design group to work on future releases of NCSA Telnet.

NCSA DataScope

Tim Krauskopf also developed NCSA DataScope, which was released in December. NCSA DataScope allows the Macintosh II user to generate several types of images from scientific data, locate the values that correspond to points on the images, and apply formulas to create new datasets.

NCSA Image

Senior Programmer Thomas Redman worked with SDG Programmers Bernhard Damberger and Dave Whittington to produce NCSA Image

You're reading an award winner!

NCSA's two newsletters—***access*** and ***data link***—shared an award at the 1988 ACM SIGUCCS User Services Conference (SIGUCCS is Special Interest Group for University and College Computing Services). In the category for newsletters over 16 pages, ***access*** and ***data link*** were awarded second place for editorial content.

Above. The NCSA Software Development Group.

for the Macintosh II (formerly NCSA ImageTool) Version 2.0. An extremely versatile application, NCSA Image uses color, contour plots, three-dimensional plots, and XY graphs to visualize scientific data, and allows palette manipulations and substitutions, multiple image viewing, and animation of sets of image frames. The original Sun version, developed largely by Research Assistant Carol Song and Research Scientist Michael Norman, is also available.

NCSA CompositeTool
Senior Programmer Mark Stupar, working with Research Scientist Barbara Mihalas, produced NCSA CompositeTool for the Sun. An exception to the highly technical, inflexible programs currently available for the production of visual presentations of two-dimensional data, CompositeTool provides a means to display, annotate, and overlay two-dimensional data—including color raster images, contour intervals of a two-dimensional data image, and vectors of two-dimensional data—in a form suitable for generating presentation-quality slides.

NCSA PalEdit
Programmer Dan LaLiberte developed NCSA PalEdit to create color palettes that may be used with other NCSA-developed software such as NCSA Image. NCSA PalEdit allows for modification of individual palette entries and the palette as a whole.

NCSA PC Show
Quincy Koziol, programmer, developed PC Show to view and manipulate color raster images on IBM PCs and compatibles. PC Show can display multiple images in sequence and permits animation of multiple image sequences.

NCSA HDF
Senior Programmer Mike Folk and Programmers Swami Natarajan and Chin-Chau Low produced NCSA HDF (Hierarchical Data Format) Version 2.0 [see page 10 and ***data link***, this issue], a multiobject file format for the transfer of graphical and floating-point data between machines.

Work in progress

In December, a number of tools began beta testing, including:

- NCSA Layout, produced for the Mac II by Programmer Rick Heintz to bring CompositeTool functionality to the Macintosh
- NCSA Image, in a new and enhanced version

Meanwhile, Programmer Dave Thompson is constructing NCSA X Image, a data analysis tool that combines features of NCSA DataScope, NCSA Image, and NCSA PalEdit in an X-window environment.

Project Leaders Eng-Whatt Toh and Dave McNabb are planning and organizing future visualization projects. Dave McNabb is concentrating on the RIVERS project [see ***access***, May-June 1988], investigating alternative paths to run-time imaging, monitoring, and steering of simulations on the CRAY systems at the center.

What is SDG's role?

When asked what they believed to be the most important aspect of SDG's role in the scientific, computer, and general communities, group members had essentially the same responses. Tom Redman and Mike Folk summed it up: the chief goal and greatest characteristic of SDG is its commitment to the production of commercial-quality software tools—hand-in-hand with scientists and in the interests of scientists—to enhance and expedite their work. And all at no charge to the user. ▲

Industrial Program

Fifth industrial partner joins NCSA

by William H. Allen
Senior Science Writer

FMC Corporation, one of the world's leading producers of machinery and chemicals, has joined the NCSA Industrial Supercomputing Program.

In a four-year, $3.3 million agreement announced by company and university officials December 15, FMC researchers and computer managers will receive training in advanced computing technologies at the center and will conduct supercomputer-based research for the corporation. The agreement becomes effective February 1, 1989.

FMC, which last year had $3.2 billion in sales, is the fifth major corporation to join NCSA's program. Other partners are Eastman Kodak Company, Amoco Corporation, Eli Lilly and Company, and Motorola Inc.

FMC, headquartered in Chicago, is one of the world's leading producers of machinery and chemicals for industry, government and agriculture. The company operates 89 manufacturing and mining facilities in 25 states and 14 foreign countries.

John A. Stevenson, coordinator of the NCSA Industrial Supercomputing Program, said the partnership with FMC will lead to further success in accomplishing one of the center's major goals—to help American industry adopt computational science and engineering methods.

"I am very pleased about the addition of FMC to our Industrial Supercomputing Program," Mr. Stevenson said. "This partnership will bring some of FMC's top researchers from throughout the company to work in our comprehensive, state-of-the art computational environment, as well as the productive intellectual environment of our Interdisciplinary Research Center. We are building a tremendous team of corporations."

Dan Irwin, FMC vice president for manufacturing and information services, said, "Participating in this program offers FMC a unique opportunity to explore the capabilities of supercomputing technology and, with assistance from the university, gain a better understanding of the benefits of supercomputing for our businesses." ▲

Software

Helping scientists share data

by Mike Folk
Senior Programmer

The NCSA Software Development Group [see page 8] has developed a file format that makes data easier to port across machines and applications. It is called Hierarchical Data Format (HDF).

HDF was created to serve the needs of NCSA's diverse scientific users, who are working on supercomputing projects of many kinds. Researchers commonly generate and process datafiles on several different machines, use different software packages to process files, and share datafiles with others who use different machines and software. HDF enables researchers to share data and to move data from one machine to another efficiently and easily.

In a typical example of the use of HDF, Scientist A wants to store a large, three-dimensional array and the results from an experiment—all in one file. Then Scientist B wants to store a copy of the data in her own file, together with two raster images created from some of the data in the original array. She might also want to include a note describing who and where the original data comes from, how the raster image was created, and other pertinent information.

Much of NCSA's software, such as NCSA DataScope and NCSA Image, now uses HDF files as a standard format for sharing data among different machines and programs.

For more detailed information about HDF, see this issue of ***data link***. ▲

Applications software on the NCSA Cray systems

NCSA's transition to the UNICOS operating system has greatly affected applications software at the center. Software availability changes day by day as applications are installed on both Cray systems running UNICOS.

So far, more than 27 applications have been installed on the CRAY X-MP running UNICOS and 44 on the CRAY-2. Already scheduled for installation are 46 more applications on the CRAY X-MP and 22 more on the CRAY-2—mostly before the end of April.

You will receive an ***access supplement*** with each of the next three newsletters to provide our current software list.

The ***supplement*** you've received along with this issue of ***access*** lists software currently installed and scheduled for installation on the CRAY X-MP system running CTSS, the CRAY X-MP running UNICOS, and the CRAY-2 system.

CRI sponsors CRAY-2 event at Beckman

To celebrate the successful installation of the new CRAY-2 system at NCSA, Cray Research Inc. sponsored a gala "event" at the newly opened Beckman Institute.

Left. Larry Smarr, director of NCSA, and Steve Griffin, staff associate, Centers Program, National Science Foundation.

Above. Morton Weir, UIUC chancellor, and Ken Bishop, NCSA visitor and professor of petroleum engineering from The University of Kansas.

Above right. Randall von Liski, director of Management Information Systems, Office of the Governor of Illinois, and Lloyd Hodges, NCSA associate director for planning and policy.

Above. UIUC administrators Dick Margison, associate vice president for business and finance; Walt Tousey, associate vice chancellor for academic affairs; and Judith Liebman, vice chancellor for research.

Above. Mike Smith, NCSA assistant director for systems, and Ted Brown, director of the Beckman Institute.

UNICOS update

by Scott Lathrop, Assistant Director, User Services

NCSA's migration to UNICOS is proceeding rapidly. We are working in conjunction with a set of friendly users to create a full software environment and to identify and eliminate as many problems as possible before production begins. The timeline below indicates our current UNICOS schedule.

January	**23**	CRAY-2 production began
February	**1**	CRAY X-MP/UNICOS transition began—UNICOS available 6 hours each weekday
	1	Applications due for March Peer Review Board (PRB) or Small Allocations Committee (SAC) for both CRAY-2 and CRAY X-MP systems
	20–23	UNICOS New User Training
March	**6–10**	UNICOS Academic Affiliates Training
	20–23	UNICOS New User Training
April	**17–20**	UNICOS New User Training
May	**1**	Applications due for June PRB or SAC
	4	CTSS production ends at 3:00 A.M.
	4	Full UNICOS production begins on the CRAY X-MP system

The CRAY X-MP transition period began February 1 with 6 hours of UNICOS production time each day. We plan to add 3 hours each day of UNICOS production time every 3 weeks. Based on user demand, we may accelerate the availability of UNICOS time. If you need more UNICOS time, please let us know by contacting the NCSA consulting office [see **NCSA Contacts** page 19].

CTSS will continue to be available on the CRAY X-MP system until May 4 to ensure that all users have time to convert their codes. All conversions *must be completed by then* since CTSS will *not* be available after May 4.

All users are receiving the NCSA *UNICOS Migration Guide* to aid in the process of converting from CTSS to UNICOS. All users are also receiving the NCSA *UNICOS Startup Package*, which contains basic information for using the UNICOS systems at the center as well as reference materials. If you need additional assistance, please contact the NCSA Consulting staff at (217) 244-1144 or Dave McWilliams, manager of academic consulting [see **NCSA Contacts** page 19].

This issue's ***access supplement*** lists the status of applications software available as of January 25, 1989. Notice of specific changes will be made through the news facility on UNICOS. Enter `man news` on UNICOS machines for information on using the news facility. ▲

NCSA Advisory Committee meets

by Jim Bottum, Deputy Director

The recently formed NCSA Advisory Committee [see box] met on December 8 to discuss policies and directions for the center as it enters a new five-year phase. The committee discussed NCSA's five-year Renewal Proposal, which had just been submitted to NSF, and also broader scientific, technological, and management issues.

Among the concerns raised by members of the committee were:

- changes in the national centers' missions, as proscribed by the National Science Foundation
- the critical role of NCSA in fostering pioneering academic research
- what constitutes a fair share of NCSA resources for industrial partners, given their level of support for the center
- the importance of continued availability of supercomputers to novice users
- whether established users should be weaned from what might be a disproportionate use of resources
- adequate space and computing resources to support distinguished visiting researchers
- equipment upgrade strategies, given inevitable budgetary constraints

Members of the Advisory Committee were selected based on their experience with computing applications and facilities management in advanced research environments. As NCSA Director Larry Smarr stated in his opening remarks, "We are trying to take a deep look at what is needed to establish a permanent national supercomputing infrastructure. We want to continually renew the manpower pool of both universities and industry—to continually create new applications of computer technology. We must never again allow this country to get in the situation we saw in the early '80s where academic researchers in America were all but cut off from access to large-scale computational resources."

In response to its charge, the Advisory Committee formulated a number of resolutions. A report on the meeting, including recommendations to NCSA in the areas listed above, is being drafted for committee comment and approval. ▲

Advisory Committee members

Kenneth Bishop. *Academic Affiliate Representative.* Professor of Petroleum Engineering, The University of Kansas.

Jonathan Dantzig. Associate Professor of Mechanical Engineering, University of Illinois.

Ernest Davidson. Professor of Chemistry, Indiana University.

Ron Deiss. *Committee Chairman.* Deputy Director, NASA Ames Research Center.

Charles Evans. Research Fellow, Theoretical Physics. California Institute of Technology.

Arthur Freeman. Professor of Physics, Northwestern University.

Eric Jakobsson. Associate Professor of Bioengineering. University of Illinois.

Lawrence Landweber. Professor of Computer Science, University of Wisconsin.

Bernard O'Lear. Manager of Systems, National Center for Atmospheric Research.

Larry Ray. *NCSA Industrial Program Representative.* Research Scientist, Eastman Kodak Co.

John Steele. Director, Computing Center, Purdue University.

Karl-Heinz Winkler. Director of Numerical Applications, Applied Theoretical Physics, Los Alamos National Laboratories.

Robert Wolff. Senior Research Scientist, Applications Technology Department, Apple Computer.

December PRB meeting

by Patricia Wenzel, Manager, User Administration

The joint NCSA/Pittsburgh Supercomputing Center (PSC) Peer Review Board held their quarterly meeting at the National Science Foundation in Washington, DC on December 15. The PRB reviewed 60 proposals, which was 50% more than at the September meeting. Of the 60 proposals, 28 were from NCSA and 32 were from PSC. Three new board members were introduced, and the Board heard brief remarks from Tom Weber, the new head of the NSF Division of Advanced Scientific Computing.

DASC Director Weber

In September 1988, Tom Weber was named Director of NSF's Division of Advanced Scientific Computing (DASC) within the Computer and Information Science and Engineering Directorate. DASC has been encouraged by the National Science Board to increase the involvement of NSF program directors in allocating time at the five supercomputer centers. Dr. Weber and his staff are currently examining various ways to accomplish this. For users and the centers, this means a change in allocation procedures and likely a return to the allocation mechanism used until 1987, whereby both NSF and each center granted allocations. Dr. Weber is asking the centers and their boards to provide their insights and comments on how best to implement this directive. NCSA welcomes input from its users on this subject.

PRB allocation statistics

Number of NCSA proposals	**28**	
CRAY X-MP only	11	
CRAY-2 only	9	
CRAY X-MP and CRAY-2	8	
Not allocated	7	25%
Partially allocated	7	25%
Fully allocated	14	50%
	X-MP	CRAY-2
Hours Requested	5812	11530
% allocated	59%	38%

Principal investigators and their approved projects

Robert Beddini, University of Illinois at Urbana-Champaign, *Analysis of Gas-Dynamic Interactions with Intense Optical Beams.* CRAY X-MP/48.

Bruce F. Carroll, University of Florida, *Computation of Confined Shock Wave Turbulent Boundary Layer Interactions.* CRAY X-MP/48.

David Ceperley and **Richard Martin,** University of Illinois at Urbana-Champaign, *Electronic Structure of Condensed Matter.* CRAY X-MP/48 and CRAY-2.

Ronald E. Cohen, Naval Research Laboratory, *Lattice Dynamics and Electron-Phonon Interaction in High Tc Superconductors.* CRAY-2.

Monical Olvera de la Cruz, Northwestern University, *Linear and Circular Polymer Gel Electrophoresis Studies.* CRAY X-MP/48.

Charles Evans, California Institute of Technology, *Numerical Relativity and Relativistic Astrophysics.* CRAY X-MP/48 and CRAY-2.

Art Freeman, Northwestern University, *Electronic Structure and Properties of Bulk Solids and Surfaces* and *Materials Research Center.* CRAY-2.

David Hoffman, Joel Spruck, and **Bruce Turkington,** University of Massachusetts *Nonlinear Problems in Mathematics and Physical Sciences.* CRAY X-MP/48 and CRAY-2.

Icko Iben, University of Illinois at Urbana-Champaign, *Stellar Structure and Evolution.* CRAY X-MP/48.

Walter Johnson and **Jonathan Sapirstein,** University of Notre Dame, *Weak Interactions Effects in Heavy Atoms.* CRAY X-MP/48 and CRAY-2.

Arieh Konigl, University of Chicago, *Two-Dimensional Simulations of Radioactive Supersonic Jets.* CRAY X-MP/48 and CRAY-2.

Susan Lamb, University of Illinois at Urbana-Champaign, *3D Smoothed Particle Hydrodynamics.* CRAY-2.

Dimitri Mihalas, University of Illinois at Urbana-Champaign, *Studies of Stellar Envelope Opacities and Nonlinear Radiation.* CRAY X-MP/48 and CRAY-2.

Gerhard Muller, University of Rhode Island, *Static and Dynamic Properties of Quantum and Classical Spin Systems.* CRAY X-MP/48.

James M. Phillips, University of Missouri at Kansas City, *The Structure of Multilayer Films near Transitions.* CRAY-2.

David N. Seidman, Northwestern University, *Molecular Dynamics Simulations of Ion Beam Induced Solid-State Reactions.* CRAY X-MP/48 and CRAY-2.

Harrell Sellers, University of Illinois at Urbana-Champaign, *Catalysis of Oxidation of Methane.* CRAY-2.

Wei Shyy, University of Florida, *A Unified Methodology for Momentum / Heat / Mass Transfer.* CRAY X-MP/48.

Robert Stein, Michigan State University, *Solar Magneto-Convection and Oscillations.* CRAY-2.

Jochem Wambach, University of Illinois at Urbana-Champaign, *Fragmentation in Nuclear Heavy Ion Collisions.* CRAY X-MP/48.

NCSA encourages and welcomes researchers to submit proposals for CRAY X-MP or CRAY-2 time. Requests for 100 hours or more are reviewed quarterly by the PRB. Smaller requests are reviewed monthly by the Small Allocations Committee.

The next PRB meeting will be in March. NCSA must receive applications by the first of the month preceding each meeting. May 1 is the deadline for the June meeting, August 1 for the September meeting, November 1 for the December meeting, and February 1 for the March meeting.

If you have any questions about allocations, please contact Patricia Wenzel [see **NCSA Contacts** page 19]. ▲

PRB members

as of December 15, 1988

Jerzy Bernholc. Physics, North Carolina State University.

David Beveridge. Chemistry, Wesleyan University.

Charles L. Brooks III. Chemistry, Carnegie-Mellon University.

Ray Chin. Computational Mathematics, National Science Foundation.

Michael Creutz. Physics, Brookhaven National Laboratory.

Kelvin Droegemeier. Meteorology, University of Oklahoma.

Richard Honzatko. Biochemistry, Iowa State University.

Piet Hut. Astrophysics, Institute for Advanced Studies.

Barry Klein. Condensed Matter Physics, Naval Research Laboratory.

H. B. Schlegel. Chemistry, Wayne State University.

Robert Swendsen. Physics, Carnegie-Mellon University.

Robert Taylor. Civil Engineering, University of California at Berkeley.

Timothy Trick. Electrical Engineering, University of Illinois at Urbana-Champaign.

Paul Woodward. Astronomy, University of Minnesota.

Computational chemistry users group hosts meeting

by Sam Milosevich, NCSA Industrial Consultant
and Kathleen Robinson, Science Writer

Dr. Warren Hehre, of the University of California at Irvine, spoke to the NCSA Computational Chemistry Users Group in December about the role of computational simulation in the development of new chemical theories.

Simulations instead of wet labs?

Discussing the possibility that simulations may eventually replace wet lab experimentation, Dr. Hehre identified two obstacles preventing broader application of these approaches.

The first obstacle is the need for vast computational resources available to each scientist, somewhat akin to having a supercomputer for each lab. The second problem lies in the development of efficient codes. Speaking of the need to go beyond old codes developed for VAX-class systems (where I/O and CPU speeds were similar), Dr. Hehre challenged scientists to develop new algorithms for the current generation of very high-speed CPUs burdened by relatively slow I/O rates.

SPARTAN

Dr. Hehre described his program, SPARTAN, which is still under development. This unique program relies on distributed functionality (relatively separate modules for user or program interface, data archives, and various computational programs) to solve the quantum mechanical equations for determining the electron structure of molecules.

One computational method described by Dr. Hehre solves quantum mechanical equations by combining the conventional precalculation and storage of integrals on disk with the Direct SCF method, which avoids disk access by recomputing integrals on each iteration. This new, combined approach precalculates the integrals, but stores them in memory in a compressed format. SPARTAN is limited by available memory, but a 256 MB memory is sufficient for most 150-basis functions.

Chemistry *continued on page 16*

***Chemistry** continued from page 15*

SPARTAN is designed to provide several modes of access. A traditional interface handles the usual z-matrix input and printed output. A new, interactive graphics interface provides interactive molecule building and graphics output of models, molecular orbitals, and electron density maps. The program interface provides automated access to the system from other computer programs.

NCSA Computation Chemistry Users Group

Approximately fifty NCSA corporate affiliate scientists, UIUC staff and students, and center staff attended the meeting, which was organized by Dr. Harrell Sellers of the NCSA Computational Science Group.

For information about the Computational Chemistry Users Group, contact Harrell Sellers [see **NCSA Contacts** page 19]. ▲

Scientific visitors

Philip E. Hardee.
December 13–17 from University of Alabama at Tuscaloosa. Area of research: astrophysics.

Nicholas Kazarinoff.
December 14–17 from State University of New York at Buffalo. Area of research: mathematics.

Theodorus Koupelis.
December 13–17 from University of Alabama at Tuscaloosa. Area of research: astrophysics.

NCSA Parallel Processing Program expands services

by Michael Welge, Manager, Parallel Processing Program

NCSA is enlarging its role in supercomputing research and development through its Parallel Processing Program. This program provides scientific researchers and computer scientists with experimental and production access to a variety of parallel architectures, enabling them to explore parallelism by experimenting with their existing applications codes, developing new codes, and evaluating execution performance.

Since its beginning in 1985, NCSA has provided its users with access to the very fast multiprocessors of Cray supercomputers. More recently, NCSA began providing access to the clustered processors of an Alliant FX/8. The NCSA Parallel Processing Program now supports 25 user projects. All of NCSA's in-house research scientists are using the Alliant FX/8 in their experiments.

Results of the experiments on clustered processors—as well as recent developments in advanced architectures and algorithms—are presented each spring at the NCSA Numerical Applications Seminar. The first seminar was held May 5–6, 1988 [see ***access*** July–August 1988], and the 1989 seminar is scheduled for May 8–10. The 1989 seminar features an enlarged scope and sports a new name, the Conference on Parallel and Vector Processing. Registration information was sent with the last ***access***, but if you need more information, contact Michael Welge [see **NCSA Contacts** page 19].

Joint project with Argonne

A vital component of the Parallel Processing Program is the interaction between two established computing centers—NCSA and Argonne National Laboratory's Advanced Computing Resource Facility (ACRF). Each center brings its own specialized expertise to this joint project. Together the two centers provide their academic and government researchers access to a wide variety of experimental architectures. This innovative plan enhances the relationship between the two computing centers and extends NCSA's parallel "platform" from multiprocessors (Cray systems) and clustered processors (Alliant FX/8) at NCSA to massively parallel and experimental architectures at ACRF.

ACRF's expertise in portable software, parallel language development, and parallel programming methodologies provides participating researchers with experimentation and development opportunities on ACRF's latest parallel architectures. These systems include: Alliant FX/8 (8 processors), AMT-DAP (1024 processors), Ardent Titan (4 processors), Encore Multimax (20 processors), Intel iPSC Hypercube (32 processors), Intel iPSC Hypercube (16 processors with vector capability), Sequent Balance (24 processors), and Thinking Machines CM-2 (16,384 processors).

NCSA, a leader in interdisciplinary computational science and visualization, provides access to its Alliant FX/8 and CRAY-2 systems. NCSA also is administering the project: distributing applications, conducting peer and project review, and coordinating training.

Vendor collaboration is important to the project. Participating vendors allow researchers access to their latest experimental machines. Access to these machines will be governed on an individual basis by the participating vendor.

From ILLIAC IV to CEDAR to Beckman Institute

The University of Illinois is widely known as the cradle of the parallel processing revolution. This tradition is supported by an intellectual environment for parallel processing that fosters advancements. Over twenty years ago, the 64-processor ILLIAC IV system was designed at UIUC. Today, UIUC continues its rich tradition of developing parallel architectures, software, and applications through its two national supercomputing centers—the Center for Supercomputing Research and Development (CSRD) and the National Center for Supercomputing Applications (NCSA)—and soon through the Arnold O. and Mabel

M. Beckman Institute for Advanced Science and Technology.

At CSRD, 70 computer scientists and electrical engineers—inspired by their director David Kuck and associate directors Duncan Lawrie, Mike Farmwald, and Ahmed Sameh—are demonstrating that high-speed parallel computation is practical across a wide range of applications. Their research is based, in part, on algorithms, architectures, and software developed at UIUC since the late 1960s. CSRD researchers are building the CEDAR parallel system, an experimental multiprocessor consisting of clusters of 8 processors, and a hierarchical memory system. CSRD is the definitive resource for information on parallel hardware and software, having hosted 25 joint seminars with NCSA and having published and presented nearly 150 papers on the topic since 1985.

The Beckman Institute, which opened in December, provides a facility for interdisciplinary research that will be conducted along parallel lines. One focus will incorporate research in biology, behavior, and cognition. Another will concentrate on materials science, computers, and computation. Projects in these interdis-ciplinary research areas will make advancements in parallel processing, both in carbon-based and silicon-based life forms.

Who's who in the program

The NCSA Parallel Processing Program is coordinated by Michael Welge, who is also project leader for clustered parallel environments. Jack Dongarra, director of ACRF, is the leader for the experimental machines. The Cray multiprocessing environment will be led by John Larson, formerly of Cray Research Inc. The project leader for the massively parallel group should be in place by summer.

Resources will be allocated through a peer review process based on formal merit review and will be subject to resource availability at NCSA and Argonne.

For more information about parallel processing at NCSA or for an application for resources, please contact Michael Welge [see **NCSA Contacts** page 19]. ▲

MEDnet offers computational tools to health care professionals

by Frank A. Wrestler, M.D., Director of MEDnet
and David P. Lawrance, M.D., Assistant Director of MEDnet

MEDnet is an innovative medical program focusing NCSA's advanced computational resources on a broad range of health care problems. Initiated in July 1988, MEDnet applies NCSA's demonstrated strengths in visualization, networking, integrated software development, and education to clinical imaging and information research.

MEDnet is offering state-of-the-art computational technology and methodology to health care professionals at local, regional, state, and national levels. Committed to multidisciplinary involvement, MEDnet is the hub of interaction for professionals in such fields as medicine, allied health, health care administration and policy, art, and theoretical and applied sciences.

MEDnet's current goals are to:

- establish a world-class center that supports the research and development of supercomputing, advanced computational technologies, and methodologies for clinical problem solving.
- provide a research environment for multidimensional image processing and information display.
- study the capture, transmission, archiving, and retrieval of patient care data.
- evaluate the social impact of supercomputer technology in health care from both provider and consumer perspectives.

Support from Apple

Apple Computer Inc. has donated six Macintosh II computers and LaserWriters to MEDnet for investigating an integrated computer platform for clinical settings.

MEDnet is conducting a national survey of medical software developers for applications that run in a Macintosh environment.

Broad academic and medical participation

MEDnet is currently supported by several University of Illinois departments on both the Urbana-Champaign and Chicago campuses, by the UIUC McKinley Health Center, and by the

MEDnet *continued on page 18*

Above. Part of the MEDnet team working in the IRC. Left to right: Kathy Vance, David Lawrance, Frank Wrestler.

***MEDnet** continued from page 17*

Champaign County (Illinois) Medical Society. As the MEDnet project develops, additional participants and project proposals will be reviewed.

Current MEDnet staff include Director Frank A. Wrestler, M.D., Ph.D.; Assistant Director David P. Lawrance, M.D., M.C.S.; Research Director William A. Airth-Kindree, M.D., M.C.S.; and Kathleen Vance, M.B.A.

To learn more about this exciting project and its new opportunities for collaboration, contact MEDnet Director Frank Wrestler by sending electronic mail to med@ncsavmsa (BITNET) or to med@ncsaa.ncsa.uiuc.edu (Internet). ▲

Selected upcoming meetings at NCSA

NCSA Second Conference on Parallel and Vector Processing
May 8–10, 1989
Jumer's Castle Lodge, Urbana, Illinois
For more information, telephone Pat Franzen, program secretary, at (217) 333-2883.

1989 NCSA Summer Institute
June 19–30, 1989
NCSA, Champaign, Illinois
NCSA is now planning its annual summer institute. Announcements with details about the institute will be sent to all users. If you are not on the NCSA newletter mailing list, telephone Kendra Reasor at (217) 244-1100 to receive an announcement.

NCSA Contacts

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the NCSA newsletter

March–April 1989 vol. 3 no. 2

Science

Young collaborator from Cornell

by Kathleen Robinson and Fran Bond

Imran Hashim is a talented senior in applied physics at Cornell University studying under Dr. Stuart Shapiro, professor of physics and a researcher at the Cornell Theory Center. Mr. Hashim was awarded a travel stipend for outstanding work as a research assistant by the Cornell Undergraduate Research Foundation. He chose to spend a week with NCSA's Scientific Visualization Program, working on techniques for visualizing the flow of a fluid past black holes.

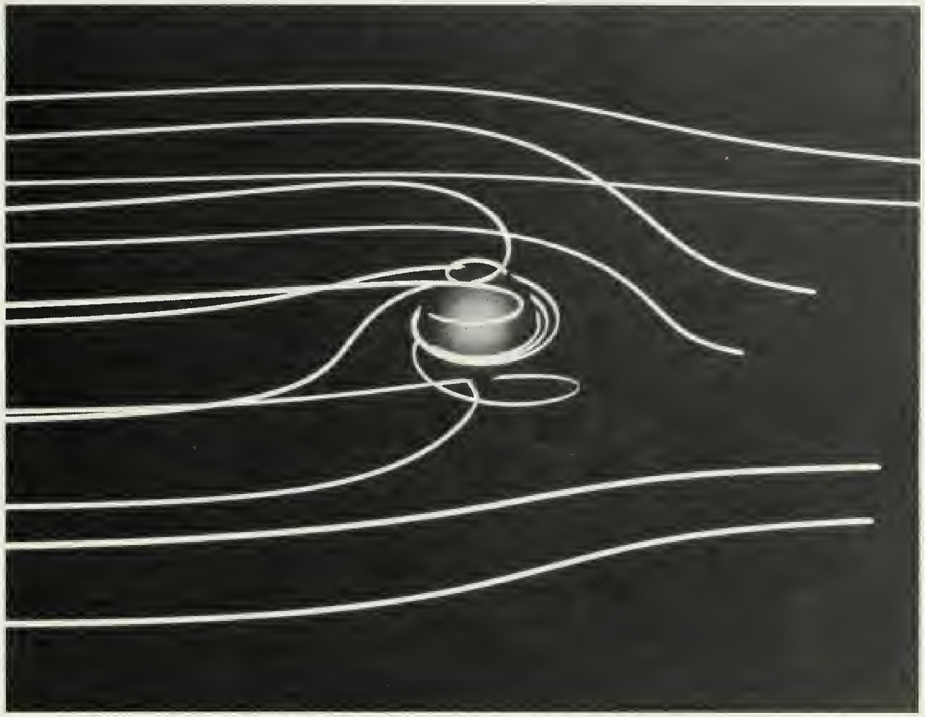
As a student research assistant on the animation team at Cornell's Theory Center, Mr. Hashim was particularly interested in NCSA because of the effective software it has developed, and because of NCSA's success with some visualization software that Cornell's center recently acquired.

It was a very busy week. Mr. Hashim worked primarily with Jeffery Yost, NCSA scientific animator, to get the equations he brought with him to the rough video stage. Also, Mr. Hashim met some NCSA general relativity researchers including NCSA Director Larry Smarr, Associate Research Scientist Roger Ove, Post Doctoral Research Associate David Hobill, and Graduate Research Assistant David Bernstein.

Cornell data, NCSA pictures

While at NCSA, Mr. Hashim generated data remotely for his project using Cornell's supercomputer, an IBM 3090. That data was then visualized running NCSA's Alliant VFX/80 with Wavefront Technologies Graphic Software and specialized software for three-dimensional surface contouring that was developed at NCSA.

***Collaborator** continued on page 3*



Above. Stream lines for fluid flow past a Kerr black hole.

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NCSA encourages researchers to submit proposals on the Crays. *See "March Peer Review Board meeting," page 14.*

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*Note: Italicized titles indicate boxed information. Since boxes are fillers, their subjects may not follow the topics of the heads under which they fall.

An apology

On page 1 of the last ***access***, one person was incorrectly identified. William Weisburg, Carl Woese's former student now with Gene Track Systems in Framingham, MA, is pictured on the right *instead of* Jordan Konisky, codirector of the Center for Prokaryote Genome Analysis.

We regret the error.

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Abbreviations

CRI	Cray Research Inc.
IRC	Interdisciplinary Research Center of NCSA
NCSA	National Center for Supercomputing Applications
UIC	University of Illinois at Chicago
UIUC	University of Illinois at Urbana-Champaign

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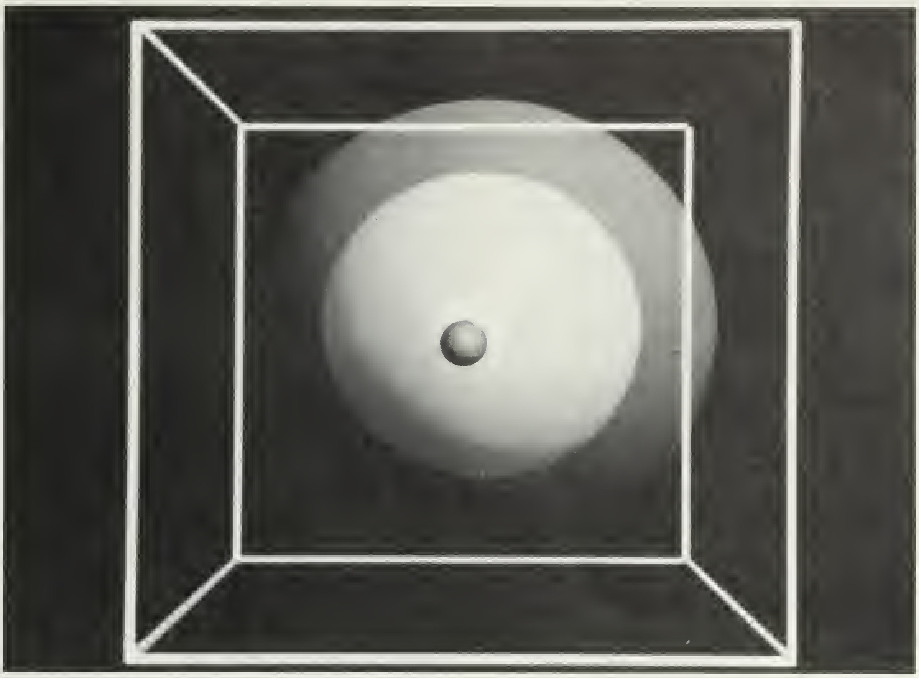


Right. Density plot for accretion onto a black hole.

Collaborator *continued from page 1*

Mr. Hashim studied two problems in his week at the IRC. The first involved accretion onto non-rotating and rotating black holes—Schwarzschild and Kerr black holes, respectively.

The second problem Mr. Hashim studied was the flow of a gas (satisfying the equation $P = \rho$, where P equals pressure and ρ is the energy density) around Kerr black holes. Cornell physicists Stuart Shapiro, Loren Petrich, and Saul Teukolsky constructed the solution, one of the rare problems in general relativity for which an analytic solution has been discovered.

Mr. Yost used code he had written to display the Lorenz Attractor [see ***access***, November-December 1988] for tracing out the flow fields around the black hole, then used other techniques to reveal the full three-dimensionality of the flow lines.

Seeing large-scale analytic solutions visualized is a major advance for scientists. Visualization is "a great step for numerical general relativists," says Mr. Hashim. "Scientists who talked for years about these problems can finally see them in full detail." David Bernstein, graduate researcher, explains, "The essential thing that is changed in the head of the scientist who sees a solution visualized is his intuition about complex events in nature. This is extremely important because intuition is most always a scientist's number one tool when making decisions about problem solving. . . . It is only a matter of time before more theoretical scientists will begin to employ modern computer graphics as a visualization tool."

Collaboration between centers

Because NCSA has developed its Scientific Visualization Program to an advanced level, visualization appears to be a fruitful area for collaborating with other centers.

At Cornell, images are generated on a Silicon Graphics IRIS workstation. The Cornell team just recently started using Wavefront software, and they are working on specialized routines to fit the software into their environment. Mr. Hashim took copies of NCSA's three-dimensional contouring program and the Lorenz Attractor code back to Cornell, as well as a ten-minute videotape of the numerical solutions. According to the visitor, the videotape produced at NCSA gave particularly good clarity and resolution.

Commenting on increased collaboration between national supercomputing centers such as NCSA and the Cornell Theory Center, Mr. Hashim remarks, "I think it benefits the scientists and staff at both places." Mr. Yost welcomes cooperation between the two centers and says he "got a better feeling for the differences and similarities of the visualization setups in both centers."

Bright future

"It is rare to see someone with expertise in both a specialized discipline of science and high-end visualization software," says Dr. Hobill, an NCSA numerical relativist,"*and* rarer still to see an undergraduate with expertise in even one of those areas. If more students like Imran are entering graduate school with such a foundation, the future of computational science looks very bright."

As for Mr. Hashim's immediate future, he plans to enter graduate school next fall. He is considering studying numerical relativity at the UIUC's department of physics because of the quality of the physics faculty as well as that of NCSA's researchers in numerical relativity. ▲

NCSA users make presentations at CRI's symposium

by Robert B. Wilhelmson, Research Scientist

Cray Research Inc. held its fourth Science and Engineering Symposium in Minneapolis, Minnesota from October 12 to 14, 1988. This symposium provides a forum for discussing recent progress in advanced scientific and engineering computing and for assessing opportunities and requirements for new applications of advanced computing systems. Thirty-one talks were given in a wide variety of application areas, with special emphasis on multiprocessor and distributed applications.

Three of the presenters were users of the NCSA computing system. Bob Wilhelmson is a research scientist at NCSA and a professor in the UIUC atmospheric sciences department; Jonathan Dantzig is an associate professor in the UIUC mechanical engineering department; and Bob Haber is an adjunct faculty member at NCSA and an associate professor in the UIUC theoretical and applied mechanics department. The papers presented appear in the *Proceedings of the Fourth International Symposium on Science and Engineering on Cray Supercomputers*, which is available from Cray Research Inc. All three presenters used videotapes in their talks.Videotapes have become a standard for the excellent presentations typically made at the symposium.

The talks by Drs. Wilhelmson and Haber included the first live, real-time visual (and interactive) displays of computations at a Cray symposium.

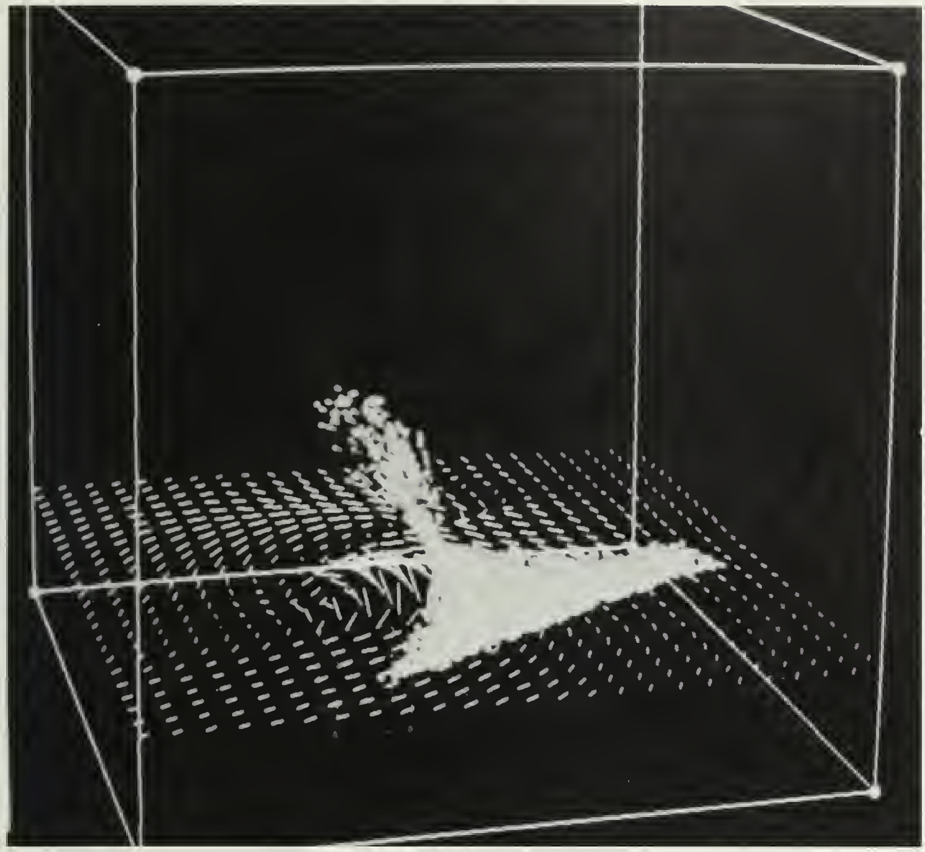
Simulating tornadoes

Dr. Wilhelmson's topic was "Numerical Simulations of Severe Storms" [see ***access***, September–October 1987]. He reviewed the history of storm modeling and presented several techniques his research group uses to visualize storm behavior. Visualization is a challenging part of studying storms, as the minimum set of equations (9) coupled with three spatial dimensions and the time dimension yields a 13-dimensional data system.

The visualization technique highlighted in the presentation involved the use of weightless tracer particles flowing through the storm model domain (the three-dimensional spatial volume in which the equations are solved). This was accomplished live on-stage using the Stellar GS1000 graphics supercomputer and the CRAY-2 supercomputer system at Cray Research Inc., which was about 10 miles away. The CRAY-2 system integrated the model equations and computed particle trajectories as the computation proceeded. The Stellar system was used with an X Window System interface to *interactively* specify particle location, color, size, and other information. The tracers were displayed in the model domain, which could be rotated while the tracers were being moved, to get a three-dimensional perspective on the particle movement, including the trails left by a selected number of particles. New trajectories could be spawned at any time from random particles distributed in a box whose size, location, and number were controlled by Dr. Wilhelmson.

The Stellar and CRAY-2 systems were linked over a T1 satellite and Ethernet network (provided by Cray Research Inc.) using sockets, a method available in UNIX for communicating between processes. The prototype software on the Stellar was developed at Stellar Computers Inc. in collaboration with Dr. Wilhelmson's storm research group (Lou Wicker and Crystal Shaw). The actual flow was delineated using the velocities being computed rather than the instantaneous flow that could be obtained from the velocities at a single time. The ability to display data, such as particle motion, while the storm simulation is underway can play an important role in delineating model physics, monitoring simulations for errors, deciding when to alter model parameters, selecting regions to store for future analysis, and debugging model codes.

Left. Still frame from crack propagation animation using interactive animation tool developed by NCSA RIVERS Project.



Left. Flow delineated using particles (spheres) on a Stellar GS1000 graphics supercomputer. Hundreds of particles move through the velocity field in real time under user control. (Credit: Dave Kamins and Craig Upson at Stellar Research, Inc. and Lou Wicker of NCSA.)

Modeling solidification

Dr. Dantzig spoke on "Computer Modeling of Solidification Processes" and the various means for computing the movement of phase boundaries in solidifying metal systems. Many manufacturing processes use solidification—particularly in the casting industry, and it is important to be able to control the process in order to control the microstructure, which determines the final mechanical properties of the part. Supercomputers are needed for these calculations because the geometries of the metal part are often complex and the underlying phenomena are described by highly nonlinear differential equations which Dr. Dantzig has been developing methods to solve.

He also described recent work concerning the interaction of fluid flow in the melt with the solidifying interface. These complex flows are of importance for crystal growth, space processing, and conventional industrial casting. Supercomputers are needed to resolve the flow patterns and the interface positions.

Visualizing solid mechanics

Dr. Haber spoke on "Computational Technologies and Visualization in Solid Mechanics Research and Design." The talk covered several new computational techniques and reviewed applications in dynamic fracture mechanics and design optimization. Beginning with a review of moving grid finite element procedures for modeling crack growth, Dr. Haber discussed how new analysis methods coupled with supercomputers are leading to improved insights into the behavior of cracks extending in brittle materials at speeds approaching one kilometer per second. A variety of visualization techniques developed by his research group (Hyun Koh and Hae-Sung Lee) were shown for studying the elastic stress waves which drive crack growth behavior.

A highlight of the presentation was a live, on-stage demonstration of real-time, interactive animation of the crack data. Dr. Haber noted that, only one year earlier, the crack growth videotape had taken several days to generate (at three minutes per video frame) for simulation data from just one CPU hour of computation on the NCSA CRAY X-MP/48 supercomputer. Using a Sun-4 workstation with a Raster Technologies GX4000 graphics accelerator, Dr. Haber showed how the animation can now be generated directly on the workstation screen at full resolution. The high resolution image from the workstation screen was monitored by the symposium audience using a video projection system provided by Cray Research Inc. During the demonstration, the strain energy and kinetic field histories from an earlier finite element simulation on the X-MP were read into the Sun workstation. Shaded polygonal representations of this data were then rendered at animation rates using the GX4000 hardware and animation software developed by Dr. Haber's mechanics research group and the NCSA RIVERS Project [see ***access***, May-June 1988]. A user interface, developed under the NeWS window system, controls the speed and direction of the animation and the rotation, pan, and zoom of the perspective view.

Dr. Haber also described his work in methods for explicit design sensitivity analysis of structural and thermal systems. These new algorithms allow engineers to effectively predict the change in the response of a system caused by a change in the design, at a

Symposium *continued on page 24*

Computational science: an international activity

by Fran Bond, Technical Editor

There is a "worldwide surge of interest in developing national supercomputing facilities modeled on the US NSF centers," says NCSA Director Larry Smarr, reflecting on some of his recent travels.

In the early 1980s, the wealthiest European countries got into supercomputing, and supercomputing facilities have proliferated. (For example, as of December 1988 West Germany had 14 installed Cray systems; France, 19; England, 18; Switzerland, 3; and Italy, 2.) On the other hand, developed countries with more limited financial resources are just now beginning to establish such facilities. Dr. Smarr noted in a recent interview that this is happening because such countries realize "they must maintain their relative position in the global economy and international scientific culture" through supercomputing.

Efforts in Finland and Australia

Finland and Australia, two countries in the process of establishing nationwide supercomputing access, exemplify this trend. From an economic standpoint, both countries are comparable and their goals are similar, according to Dr. Smarr. Based on their much smaller national populations and financial resources (about one-tenth that of the United States), each has determined that one major supercomputing center is adequate for the country's needs.

For the first time, each country held a major conference to plan its future in supercomputing. During the last quarter of 1988, Dr. Smarr delivered the keynote address at each conference. Leaders of government, industry, and academia as well as the media turned out to both events.

Above. To illustrate her lecture at the University of Industrial Arts in Helsinki, Donna Cox included this computer art image entitled "Introspective."

Finland's topical meetings

All Scandinavia is moving toward establishing a regional computing network. Scandinavians realize that their "best minds must have access to supercomputers and they must train the next generation in supercomputer technology," said Dr. Smarr. The Finnish State Computer Centre (VTKK) at Espoo, near Helsinki, is Finland's component of the Scandinavian network. VTKK's supercomputer, located in the Centre for Scientific Computing, supports its country's academic and industrial research as well as weather forecasting.

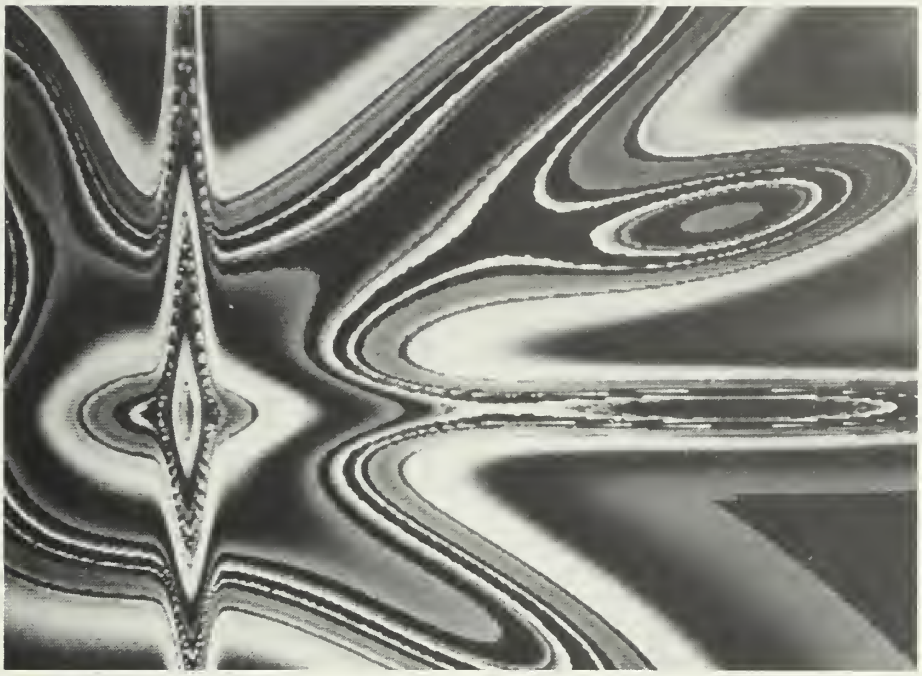
In 1987 and 1988 while Finland's supercomputing center was in the planning stage, a delegation from that country visited many US centers, including NCSA. They sought information about the organization and administration of a supercomputing center to help them make decisions about establishing their national center. Representatives of the Ministries of Finance and Education, the Finnish Meteorological Institute, the Technical Research Centre of Finland, and the Finnish State Computer Centre—who formed the Board for the Finnish Supercomputer Acquisition Project—visited NCSA. Dr. Esko Hammarén, research coordinator at the Centre for Scientific Computing at VTKK, accompanied the group. As a result of these visits to NCSA, Dr. Smarr was invited to be the keynote speaker at Finland's first supercomputing conference.

"NCSA, being one of the forerunners [of major US supercomputer sites]," said Dr. Hammarén in a recent interview, "shows a pioneering enthusiasm in many aspects typical to the second wave of supercomputing. We want to share in this spirit and action in Finland. . . . One of the major impacts of supercomputing to society will be the role of supercomputer centers within the scientific society as well as between academia and industry." Expressing special interest in NCSA's interdisciplinary efforts, he continued, "Visions opened by the Interdisciplinary Research Center of NCSA really impressed our delegates, not the least myself. We hope to be able to establish something similar in the near future. For this and other international contacts," he concluded, "the NCSA people are of vital importance."

VTKK was the site of a two-day conference in September 1988. Organized by Dr. Hammarén, this was the first in a series of four topical meetings for supercomputing in Finland. Less than a month prior to the conference, the Finnish government signed a contract with Cray Research Inc. to install a supercomputer of the X-MP class at VTKK by the year's end. This conference marked that occasion as the first day's theme signifies—"Opening of the Supercomputer Era in Finland." Dr. Smarr's keynote address was "Supercomputing, Science and Society." Associate Director and Corporate Officer John Stevenson's speech, "Supercomputing and Industry," followed. That evening Dr. Smarr gave a public lecture, "Contribution of Supercomputing to the Sciences and Society," at the University of Helsinki. While in Finland, Dr. Smarr and Mr. Stevenson met with leaders of government and industry and gave many interviews to representatives of the press and TV.

In November 1988, Donna Cox, assistant professor in the School of Art and Design at UIUC and adjunct professor for supercomputing applications at NCSA, gave the keynote address, "The Art of Scientific Visualization," at the third topical meeting on Finnish supercomputing. Also at VTKK, this conference was attended by leading mathematicians and representatives of emerging disciplines utilizing supercomputing. Ms. Cox gave a second talk on interdisciplinary applications in scientific visualization. Prior to the conference, she lectured at the University of Oulu on "The Art of Scientific Visualization" and at the University of Industrial Arts in Helsinki on "New Directions for the Industrial Artist: Collaborations in Science and Engineering." In Finland, she met leading artists, designers, and scientists. Planned as the cover story until the Armenian earthquake intervened, Ms. Cox's work and the pioneering scientific visualization at NCSA were featured in the Finnish equivalent of *TIME* magazine, *Suomen Kuvalehti*. A computer magazine, *Tietoviihho*, also highlighted NCSA in one of its issues.

Below. Donna Cox's computer art image "Implosion" shown at the University of Industrial Arts in Helsinki.



Australia's conference

During February and March 1987, two Australian research scientists visited NCSA: Drs. Geoff Bicknell of Mt. Stromlo Observatory and Robert A. Gingold of the Australian National University (ANU). As members of the NCSA Visitors Program, they worked on smoothed-particle hydrodynamics algorithm development and turbulent shear layer simulations with Associate Director and Research Scientist Mike Norman. Their experiences at NCSA helped lead to the decision to try to get consensus in Australia for getting government, industry, and academia to create a national supercomputing center. A leader in this effort has been Dr. Donald Faulkner, academic director of the Australian National University Supercomputer Facility (ANUSF), which has a Fujitsu FACOM VP100 supercomputer. At the suggestions of Dr. Bicknell, a major user of ANUSF; Dr. Gingold, a staff member at ANUSF; and others, Dr. Faulkner pulled together the first national supercomputer conference in Australia. Again, Dr. Smarr was chosen to give the conference's keynote address.

"Australia is not as far advanced as is Finland in developing a supercomputer policy and implementing a national center, but the visit of Dr. Smarr was instrumental in helping shape the thinking of the government's policy-making bodies," Dr. Faulkner commented recently. "In addition to the worldwide trend towards establishing NSF-style national centers, Australia is also seeing many of its competitor countries in the Pacific Rim region of

International *continued on page 8*

International *continued from page 7*

Asia overtake it in adapting to the new technological age." For example, he noted, South Korea and Singapore recently announced plans for establishing large national centers. "The conference attended by Dr. Smarr did much to clarify the ideas of the Australian supercomputing community on the most desirable format for government investment," Dr. Faulkner continued. "There was overwhelming support for the development of a single national center, providing the same high level of professional expertise [that] occurs at the NSF sites. Above all, there was enormous interest in the use of the visualization software that has been developed at NCSA, and this will be distributed in Australia through the ANU Supercomputer Facility."

"The Supercomputing Society" was the theme of the First Australian National Supercomputer Conference in December 1988. Held at and hosted by ANU, the aim of the three-day conference was to bring together supercomputer users and hardware vendors. "Supercomputers, Visualization, and the US Computational Infrastructure" was the title of Dr. Smarr's keynote address; later in the day he gave a public lecture, "The Supercomputing Society." Dr. Smarr was also a member of the closing panel that discussed the future of supercomputing in Australia. Barry Jones, MP, Minister for Science, Customs, and Small Business, chaired the discussion.

While in Canberra, Dr. Smarr met privately with a number of top Australian government officials. This included informal presentations to the Australian Science and Technology Council and the Australian Research meeting with officers from the Departments of Industry, Technology, and Commerce—primary government committees that deal with science and technology—to brief the Australians on the impact of establishing a national supercomputing facility. Dr. Smarr was frequently interviewed by radio and TV during the conference.

After the conference, Dr. Smarr flew to Sydney to give a colloquium on "Supercomputers and Visualization: The Impact on Our Society" which was sponsored by the Radiophysics Division, Commonwealth Scientific and Research Organisation (CSIRO). A government organization, CSIRO has in the past provided some national access to a Cyber 205. It is also the parent organization for The Australia Telescope. While in Sydney, Dr. Smarr was the guest of Dr. Ron Ekers, director of The Australia Telescope (formerly director of the Very Large Array Telescope in Socorro, New Mexico).

Following the colloquium, Dr. Smarr traveled to Narrabri in the Outback to see The Australia Telescope, the major radio telescope in the Southern Hemisphere. A six-dish array was under construction there, and Dr. Smarr talked with the antenna designers about NCSA's initiative in radio astronomy software. Following that, Dr. Smarr visited the Australian Institute of Marine Science (AIMS) at Townsville in Queensland as the guest of Director Joe Baker. AIMS is dedicated to protecting and studying the Great Barrier Reef. Dr. Smarr went on a scientific expedition out on the reef, which involved three days of snorkeling and scuba diving, to work with researchers led by Dr. Peter Moran who are studying the destructive Crown-of-Thorns starfish, a serious threat to marine life along the commonwealth's coastline.

As a result of discussions with Dr. Smarr, AIMS researchers have expressed interest in visiting NCSA to develop complex simulations of ocean flows around the reef where the starfish propagate. To work with their field data, AIMS wants to use software such as NCSA Image (formerly ImageTool) and NCSA DataScope [see ***access***, January – February 1989]. NCSA's personal computer software, such as Image and DataScope for the Macintosh, may be useful for visually analyzing ecology field data taken on the reefs. ANU will distribute the software around Australia. Before leaving Queensland, Dr. Smarr spoke at James Cook University.

NCSA's international influence

Recently reflecting on his experiences in Finland and Australia, Dr. Smarr remarked that both countries regard the NSF centers, including NCSA, as "wonderful examples of what can be done." But they can't directly transplant the NSF model to their nations, he cautioned, because the traditional interrelationships of government, industry, and academia in their countries differ from those in the United States.

"What they really like about NCSA," he added enthusiastically, is "the Interdisciplinary Research Center; having the most advanced technology in one place and *access* to it; the training that goes on here; the technology transfer between government, universities, and business; and all love the visualization" along with NCSA's concept of individual workstation software tools. "In Australia and Finland there has been little previous use of visualization," he pointed out.

In 1989, two of NCSA's major thrusts in scientific research will be in astronomical imaging and in climate and environmental threats. The former will now involve researchers at The Australia Telescope, while the latter thrust could be relevant to scientists at AIMS concerned with threats to the Great Barrier Reef. "We look forward to Australian researchers joining our modeling and simulation efforts through visits and ultimately an international network," said Dr. Smarr.

"NCSA is putting a major effort into working internationally with other countries to develop their centers," he continued. "Traditional science is inherently an international activity; computational science must become international as well." ▲

Scientific visitors

Dean Sumi.
February 3-11 from California Institute of Technology. Area of research: astrophysics.

Wen Bo Yuan.
February 10-20 from Drexel University at Philadelphia. Area of research: cosmology.

NCSA director visits Cray Operations

Seymour Cray (left) and Larry Smarr (right) outside Cray's Colorado Operations at Colorado Springs. On this visit, Dr. Smarr was one of the first people to get a tour of the new CRAY-3 supercomputer manufacturing facility. Dr. Smarr says "Every step of the process is breaking new technological ground. I was extremely impressed."

Selected upcoming meetings

Connection Machine Seminar and Workshop
April 17–18, 1989
NCSA, Beckman Institute, Urbana, IL
For more information, contact Michael Welge, workshop coordinator, at (217) 244-1999.

NCSA Second Conference on Parallel and Vector Processing
May 8–10, 1989
Jumer's Castle Lodge, Urbana, IL
For more information, contact Pat Franzen, program secretary, at (217) 333-2883.

NCSA 1989 Summer Institute
June 19–30, 1989
Pending funding from the National Science Foundation
NCSA, Computing Applications Building, Champaign, IL
For more information, contact Alan Craig, manager of training, at (217) 244-1988.

NCSA Summer Workshop on Supercomputer Education
July 10–21, 1989
Pending funding from the National Science Foundation
NCSA, Computing Applications Building, Champaign, IL
For more information, contact Nora Sabelli, workshop coordinator, at (217) 244-0644 or nsabelli@ncsa.uiuc.edu.

Massively Parallel Computing Summer Workshop
July 31–August 4, 1989
Pending funding from the National Science Foundation
NCSA, Computing Applications Building, Champaign, IL
For more information, contact Michael Welge, workshop coordinator, at (217) 244-1999.

13th Conference on the Numerical Simulation of Plasmas
September 17–20, 1989
Hilton Hotel, Santa Fe, NM
For more information, contact Mike Norman, member of Scientific Organizing Committee, at (217) 244-2006.

NCSA Users' Group Meeting
October 16–17, 1989
NCSA, Beckman Institute, Urbana, IL
For more information, contact Janice Knapp-Cordes, assistant training coordinator, at (217) 333-0085.

Profile

Interview with Roger Ove, associate research scientist

by Kathleen Robinson, Science Writer

Above. Roger Ove, associate research scientist at NCSA

Dr. Roger Ove, an associate research scientist at NCSA since June of 1987, was recently interviewed by ***access*** about his research and his role at NCSA.

Would you describe your present work in lay terms?

My research centers on an attempt to understand the structure of the Einstein equations using novel hardware. Although conceived by Albert Einstein nearly 80 years ago, the general theory of relativity is still largely not understood in the sense that the types of behavior that can be exhibited are unknown. This is because the conjectures of the theory can be attacked with pencil and paper or conventional machines only in greatly simplified cases. We are just beginning to probe the full nonlinear behavior of the theory, using computational means.

What types of questions do you and others in your field want to answer?

Does the theory allow an observer to travel backwards in time? How does symmetry influence the existence of singularities? Do families of constant mean curvature surfaces exist in various spacetimes?

We know that certain solutions to Einstein's equations which use special symmetry allow observers to travel into their pasts. A popular speculation is that if this symmetry is relaxed, such behavior will *not* be present. This point of view is part of the Cosmic Censorship Conjecture; the proof is the primary unsolved problem in relativity theory.

Relaxing the symmetry is inconceivable without a supercomputer. Traditionally, numerical simulations have not been widely employed to address such mathematical questions, since simulations do not in general provide definitive evidence. However, physical observations of nature do not provide definitive evidence for general theories of nature, yet the utility of such observations is beyond question. If computer simulations can be used to probe the validity of mathematical conjectures, we can avoid a great expense of time and effort in attempts at formal proof of false conjectures.

Could you say some more about the use of computers in studies of the Einstein equations?

The Einstein equations represent a geometrical theory of gravitation, expressed as a system of elliptically constrained nonlinear partial differential equations. The idea is to probe the structure of the solutions (spacetimes) to these equations by numerical approximation. The equations can be transformed into a very large system of ordinary differential equations with algebraic constraints, and this system can be integrated. It's not quite as simple as that, since in general this prescription will run into coordinate problems that will halt the evolution and steps must be taken to preserve the constraint conditions. Also, once such a spacetime has been generated, it is not a simple matter to extract physically relevant information.

What computer are you using in this research?

Evolving such spacetimes is a very computationally intensive procedure, and problems are made tractable by imposing a direction of symmetry. To scan a greater variety of configurations—to investigate chaos for example—it is necessary to impose *more* symmetry and additional approximations. Currently, I am working with a toy Einstein equation using a Connection Machine—a massively parallel computer from Thinking Machines Inc.—that is at NPAC, the Northeast Parallel Architectures Center at Syracuse University. Such parallel machines also offer the best hope to simulate the completely general case with no symmetry, since their performance potential far exceeds that of vector machines.

I'm also interested in improving the computational environment, to make computers better able to serve science. In general, I have more interest in tools to ensure the correctness of programs than those that enhance their performance. It is more wasteful to run a *wrong fast* program than a *correct slow* one. Of course, speed is also important, but not at the expense of sound design and structure. I am currently collaborating with a CS group at Carnegie-Mellon University (CMU) on an environment to promote such design, by providing a visual interface into the program and data structure.

A visual interface? That sounds interesting. Can you say more about that?

Phil Miller at Carnegie-Mellon and I will be developing a portable elaboration of CMU's MacGnome Genie programming environments. These programming environments are currently used for teaching computer science, but they provide a good base upon which to build a production system. They eliminate a lot of the syntactical tedium of programming by relegating that to the computer, and allowing the human to deal with the more fundamental issues of program design and structure. We want to provide the user with the same powerful environment regardless of the machine being used—even a supercomputer. The environments will also provide an excellent vehicle for bringing undergraduates into contact with supercomputers, since the students will be able to make rapid progress without having to learn the details of computer languages.

Does your work dovetail with other numerical relativity work being done at NCSA?

Most of the work being done at NCSA (by David Hobill, David Bernstein, and Larry Smarr) centers around simulating a local region of a spacetime, such as in the vicinity of a black hole. The long term goal of such work is to be able to predict the signal of gravitational radiation from realistic astrophysical events. I don't work in this area, and stick to spatially closed vacuum spacetimes—without a lot of the practical difficulties associated with boundaries and singular coordinates. It all depends on the questions you are trying to answer. I'm not attempting to model the physical universe, but rather the Einstein equations. Of course there is some overlap of interest. For example, David Hobill is doing some interesting work on the subject of gravitational chaos [see ***access,*** November-December 1988] and I have a great deal of interest in that topic.

How did you get started in this line of research?

In grad school I was toying with the idea of going into high-energy physics, with the guys who use the big accelerators like the ones at Fermilab or CERN. But you spend so much time on technology in that business, you never see the physics, so I started looking for something else. My undergraduate advisor told me that if he were doing it again he would go into astrophysics, and that there was a highly regarded astrophysicist (who will remain nameless) at Yale that I might work with. That sounded pretty good to me, so I approached my department chairman with the idea and discovered to my embarrassment that the highly regarded astrophysicist was dead. Well, there were some people working on relativity in the theory group so I turned there. I don't really have much interest in stars anyway.

My thesis advisor, Vincent Moncrief, was interested in the mathematical structure of the Einstein equations, and felt that computers might be useful in addressing the topic. Since I had some background with computers it was sort of natural, although I had to overcome a revulsion for numerical approaches. It is simply the case that certain questions can't be dealt with by any other means. There is a certain elegance in addressing problems numerically, in that one can deal with the problems at a fundamental level without a lot of the excess baggage of contrived mathematical formalisms.

What about the role of research scientists on the staff at NCSA—can you talk about that a bit?

One role of the research scientists at NCSA is to prototype ideas that make their work more productive, leaving development to those more qualified to support it. The problems and solutions illustrated by such prototypes tend to influence supported NCSA software. Lately I've been working on some network distributed applications between workstations and Cray supercomputers, to make them more usable. This work was supported by a Cray Research cooperative agreement.

From what you said earlier, it sounds like your work is heavily mathematical.

In a sense—I work on mathematical subjects, although I am by no means a mathematician. For example, the question of whether constant mean curvature foliations exist in a given Einstein spacetime is a subtle mathematical question involving the nonlinearity of both the field equations and the problem statement. The question can be stated without elaborate formalism, and it can also be *answered* without formalism. It seems to me that many physicists confuse formalisms of technique with mathematics.

Nonphysicists do too, it would seem. . . One last question—do you remember how you first got started using computers?

When I was in college it occurred to me that I didn't understand how it was possible to make a programmable machine. So I took a few courses on semiconductor electronics and computer science. Presumably my questions were answered (or maybe I forgot the questions).

Presumably—apparently—they were! ▲

UNICOS migration

by Scott Lathrop, Assistant Director, User Services

The migration from CTSS to UNICOS is nearing the final phase. **All users must have converted to UNICOS by May 4, 1989.**

If you have encountered any problems which have impacted your ability to convert, please contact us so that we may provide you with assistance. You may call the NCSA consultants or Dave McWilliams [see **NCSA Contacts**, page 23] to have a consultant assigned to work with you.

All users should have received both the *UNICOS Migration Guide* as well as the new *UNICOS Start-up Package*. If you have not received these, please let us know so that we may get copies to you by calling the main receptionist at (217) 244-0072.

Included with this mailing is a list of the applications software at the time of printing, *Applications Software on the Cray Systems*. A more up-to-date list of applications software is available online on both CRAY systems by entering `help software`. If you need further information on software availability, contact either the consultants or the Manager of Applications Software [see **NCSA Contacts**, page 23]. ▲

Training sessions

Upcoming training sessions are as follows:

1989 May 22-25
New User Training

June 5-8
New User Training

You must register at least one week before each session. To register or to get more information about the training program or one of the training sessions, contact the Manager of Training [see **NCSA Contacts**, page 23].

Scientific Visualization and Media Services Group

by Scott Lathrop, Assistant Director, User Services

The manager of the Scientific Visualization Program, Stefen Fangmeier, recently left NCSA to work for Mental Images in Berlin, West Germany. Mr. Fangmeier's efforts to make the NCSA visualization program a great success have been well appreciated.

During his time at NCSA, Mr. Fangmeier worked on a number of visualization projects, including the recent SIGGRAPH '88 tape which was presented at the SIGGRAPH show in Atlanta last August. Other productions of his include "Simulated Tornadic Storm Development," "Comparisons of the Spatial Distribution of Abell Clusters with Numerically Simulated Model Clusters," "Enzyme Reaction in Triosphosphate Isomerase," and "River Basin Water Chemistry." NCSA wishes Mr. Fangmeier well in his new position.

In order to continue to provide NCSA's users with excellent support, we have merged the Scientific Visualization Program and the Scientific Media Services (SMS) Group into a single unit, with Dan Brady, the former manager of SMS, as the new manager. Mr. Brady brings to this position excellent managerial skills and a tremendous understanding of the visualization needs of the research community.

The new group is called the Scientific Visualization and Media Services Group. Please feel free to call Mr. Brady if you have any questions about the services provided [see **NCSA Contacts**, page 23] ▲

Cumulative indexes available for 1988 ***access*** and ***data link***

Now you can locate information described in any article in volume 2 of the two NCSA newsletters, ***access*** and ***data link***—just check their cumulative indexes for 1988 which were mailed with this issue of ***access***.

To get a copy of any indexed article, simply order the back issue in which the article originally appeared. To order a back issue, call NCSA at (217) 244-0072 or use the order form in the NCSA *Technical Resources Catalog Supplement*, which also accompanies this issue of ***access***.

Lloyd Hodges, new associate director at NCSA

by Fran Bond, Technical Editor

Below. Lloyd Hodges, new associate director.

In December 1988, Lloyd Hodges joined NCSA as associate director of planning and policy. He reports directly to Deputy Director Jim Bottum.

“NCSA is growing fast, “ says Mr. Bottum. “We are double in size from where we were two years ago and the trend shows every sign of continuing. We decided it was time to institute a permanent planning function in the center to help this growth. Lloyd Hodges is the perfect person for the task because he brings a seasoned perspective to the position that includes both public and private sector experience.”

Speaking of his role at NCSA, Mr. Hodges pointed out that his real challenge is to “balance planning and creativity. We want to be able to do enough planning so that we're not wasting valuable resources,” he said; “but we don't want that planning to be so rigid that it stifles creativity.” Since NCSA's mission is facilitating scientists' ability to use supercomputing power in their research, he sees his role as one of support in that endeavor—both to the scientists themselves as well as to the entire NCSA staff in its service to users.

Immediately prior to coming to NCSA, Mr. Hodges consulted for University President Stanley Ikenberry's office on issues facing Central Administration on both the Urbana-Champaign and Chicago campuses. These issues covered a range of problems including tax liability vis-a-vis the Unrelated Business Income Tax (UBIT) laws, strategic planning for adjunct units of the vice-president's office, and an evaluation of a mainframe database management system (DBMS) for the UI Foundation.

Mr. Hodges received a Ph.D. in marketing research and psychological measurement from the UIUC's College of Commerce and Business Administration in 1982. He taught strategic management, marketing management, and marketing research at UIUC and Illinois Wesleyan University before becoming a consultant. Prior to returning to school for graduate study, he was an executive for a Fortune 500 retail food chain with responsibilities in personnel, labor relations, and training.

Of his position at NCSA, Mr. Hodges says, “It's especially challenging because this is a dynamic, creative—sometimes turbulent—environment where many problems are unique rather than recurring in nature. So it causes a planner to be constantly taking in data and creating useful information. I find this extremely challenging and stimulating, and this makes NCSA a very attractive place to work.” ▲

Joe Golab joins NCSA Computational Chemistry Group

by Sam Milosevich, Industrial Consultant

Joe Golab joined the NCSA Applications Software Group in January 1989. He is the newest member of the Computational Chemistry Group headed by Dr. Harrell Sellers [see ***access***, May–June 1988].

Above. Joe Golab, applications scientist, chemistry.

Dr. Golab's responsibility is to further develop the computational chemistry capabilities available through NCSA's library of codes and utilities. Also responsible for examining and evaluating user-developed methods and applications, he welcomes the opportunity to conduct research in collaboration with NCSA users. His own research interests are in the area of transition metal complex chemistry and the calculation of various molecular properties.

Dr. Golab comes to NCSA from a postdoctoral research position at Northwestern University with Professor G. C. Schatz, where he focused on chemical reaction dynamics and hyper-Raman scattering. At Texas A&M University, Dr. Golab obtained his Ph.D. degree under the direction of Professor D. L. Yeager in the area of electronic structure theory. He has developed, programmed, tested, and applied several ab initio codes and has experience with semiempirical techniques.

Dr. Golab is particularly pleased that NCSA is involved in a variety of areas that mix basic research and chemical applications. He suggests that he be given the chance "to wear out the phone" hearing what users want in a friendly environment for computational chemistry at NCSA.

Other members of the Computational Chemistry Group led by Dr. Harrell Sellers include Drs. Gail Golab, Sam Milosevich, Nora Sabelli, and Ms. Hui Yu. ▲

March Peer Review Board meeting

by Patricia Wenzel, Manager, User Administration

NCSA has time for allocation on the supercomputers. Researchers are encouraged to submit applications for time on the CRAY X-MP/48, the CRAY-2, or both systems. Applications for 100 or more service units (SUs) will be reviewed at the next Peer Review Board meeting in June (May 1 application deadline). Applications for fewer than 100 SUs will be sent out for external review and allocated by the Small Allocation Committee which meets monthly.

The March meeting of the joint NCSA/Pittsburgh Supercomputing Center (PSC) was held at NCSA on March 13. The board reviewed 41 proposals: 19 from NCSA and 21 from PSC.

Principal investigators and their approved projects

Marvin L. Cohen and Steven G. Louie, University of California at Berkeley, *Quantum Theory of Clusters and Solids*. CRAY X-MP/48, 730 SUs.

Jonathan Dantzig, University of Illinois at Urbana-Champaign, *Continuous Casting of Steel* and *Modeling Crystal Growth in Microgravity Environment*. CRAY-2, 195 SUs.

Rodney Douglass, University of Nebraska at Lincoln, *Bifurcating Solutions of Natural Convection in Enclosures*. Cray-2, 50 SUs.

D. Scott Eberhardt, University of Washington, *Numerical Investigation of Multiple-Species Compressible Shear Layers with Heat Addition, Numerical Simulation of Instabilities in Compressible Mixing Layers,* and *Numerical Simulation of Detonation /*

Boundary Layer Interaction. CRAY-2 and CRAY X-MP/48, 50 SUs.

Karl Hess, University of Illinois at Urbana-Champaign, *National Center for Computational Electronics.* CRAY-2 and CRAY X-MP/48, 1500 SUs.

Horia Metiu and Vincent McKoy, University of California at Santa Barbara, *Electron Scattering by Adsorbed Molecules.* CRAY X-MP/48, 150 SUs.

Daniel J. Pasto, University of Notre Dame, *Theoretical Study of Organic High-Energy Intermediate.* CRAY X-MP/48, 100 SUs.

George Schatz, Northwestern University, *Theoretical Studies of State to State Chemistry*. CRAY X-MP/48, 200 SUs.

Hugh L. Scott, Oklahoma State University, *Monte Carlo Simulation of Cholesterol in Model Membranes.* CRAY X-MP/48, 140 SUs.

Walter Wilcox, Baylor University, *Hadron Structure and Lattice QCD.* CRAY-2, 95 SUs.

Peter Wolynes, University of Illinois at Urbana-Champaign, *Advanced Computational Materials Science Thrust.* CRAY-2 and CRAY X-MP/48, 300 SUs. ▲

PRB allocation statistics

Number of NCSA proposals	**19**		
CRAY X-MP only	9		
CRAY-2 only	8		
CRAY X-MP and CRAY-2	2		
Not allocated	3	16%	
Partially allocated	9	47%	
Fully allocated	7	37%	
	X-MP	**CRAY-2**	**Both**
Hours requested	**1900**	**1430**	**2700**
Percent allocated	70%	26%	66%

CRAY-2 dedicated time

by Scott Lathrop,
Assistant Director, User Services

To promote large production jobs and multitasking, NCSA is offering dedicated time slots on the CRAY-2. In dedicated mode, all four processors and all of the available memory (approximately 122 MWords) will be available to a single job. The following guidelines are being used to establish this dedicated environment.

NCSA will provide up to four hours of dedicated time each evening on an as-needed basis. When this time is not needed, normal production runs and interactive access will continue. Dedicated time may be scheduled between 11 p.m. and 3 a.m. CST, starting later when less than four hours are requested.

Dedicated time is available in two forms: NQS queue submission and interactive access.

The NQS queue allows a user to submit a job to be run in dedicated mode when time is available. NCSA operations will schedule running these jobs as time permits with at least a half hour's worth of jobs using less than ten minutes each evening. Longer running jobs will be held in the queue until time permits running them within the dedicated timeframe. If you wish to submit NQS jobs, submit them to the dedicated queue.

The interactive access mode allows a user to log on to the system and perform his/her work. In this mode, a single user (or group of users within a project) will be allowed to log in and run jobs as he/she wishes. This mode of operation requires the user to sign up in advance for a minimum of two hours of time. It is the user's responsibility to use all of the time requested to the best of his/her ability since the time to switch the system from single user back to multi-user is rather lengthy.

If you would like to sign up for dedicated interactive time, please contact the NCSA Consulting Office [see **NCSA Contacts**, page 23] at least 48 hours in advance so that we may schedule your access around other activities.

Dedicated time will be charged based upon the amount of wallclock time used, multiplying the wallclock time by 4. Thus, a one-hour dedicated time slot will be charged 4 Service Units (SUs).

At this time, NCSA is not offering this option on the CRAY X-MP. This is a new offering at NCSA, and we would like to hear from you as to how we can improve it to allow you to better accomplish your research objectives. As we learn from our early experiences and the feedback from researchers, we will reevaluate and possibly modify this offering. ▲

MSC/NASTRAN available, courtesy of the NCSA Industrial Program

by Larry White, Assistant Director, Industrial Program

MSC/NASTRAN uses finite element methods to compute results to engineering analysis problems. Widely used by many engineering companies, MSC/NASTRAN performs static and dynamic structural analyses; analyzes material and geometric nonlinearity; and works problems in heat transfer, aeroelasticity, acoustics, and electromagnetism.

Above. Ramesh Jayaraman (left), MSC/NASTRAN user consultant, and Ilhan Dilber (right), software coordinator for engineering applications.

As one of the benefits to the center's academic users, the NCSA Industrial Program has arranged for an MSC/NASTRAN license—paid for entirely from industrial funds—which allows academic researchers to use the software for formal class work and for academic research at no extra charge. Graduate students in engineering can now be trained to use MSC/NASTRAN on the supercomputer as one of their tools in solving large-scale analysis problems. NSF and university-funded research projects can also use MSC/NASTRAN at no extra charge.

Documentation on using MSC/NASTRAN is available directly from:

MacNeal-Schwendler Corporation
815 Colorado Boulevard
Los Angeles, CA 90041
(213) 258-9111

You can order any of the following manuals. The manuals are listed in order of difficulty, from the beginning level to more complex:

- *MSC/NASTRAN Primer*
- *MSC/NASTRAN User's Manual*
- *The NASTRAN Theoretical Manual*
- *MSC/NASTRAN Application Manual*
- *MSC/NASTRAN Demonstration Problem Manual*
- *MSC/NASTRAN Verification Manual*
- *MSC/NASTRAN Handbook for Linear Analysis*
- *MSC/NASTRAN Handbook for Superelement Analysis*
- *MSC/NASTRAN Handbook for Thermal Analysis*

Additional descriptions of these documents are in the January 1989 NCSA *Technical Resources Catalog.*

If you are an academic researcher who wants to get started with MSC/NASTRAN or has questions about its use, you may contact Ramesh Jayaraman, NCSA user consultant, by telephoning (217) 244-1990 or by sending electronic mail to 13019@ncsavmsa (BITNET) or 13019@ncsaa.ncsa.uiuc.edu (INTERNET).

Happy calculating, compliments of the NCSA Industrial Program. ▲

New NCSA software releases

by Ann Stowell, Product Coordinator, Software Development Group

NCSA HDF Version 2.0
NCSA HDF, or Hierarchical Data Format, is a multi-object file format designed to facilitate the transfer of graphical and floating-point data between various machines and operating systems, including the Cray, Sun, Alliant, Macintosh, and IBM PC computers. The format allows self-definition of data content and easy extensibility for future enhancements or compatibility with other standard formats. NCSA HDF includes Fortran and C calling interfaces; utilities to prepare raw image or data files for use with other NCSA software; an interface for storing and retrieving compressed or uncompressed raster images with palettes; and an interface for storing and retrieving scientific datasets of up to seven dimensions together with information about the data, such as labels, units, formats, and scales for all dimensions. For further information, see ***data link***, January– February 1989, and this issue of ***data link***.

NCSA Image for the Color Macintosh Version 2.0
NCSA Image (formerly NCSA ImageTool) is a color-imaging application that displays 8-bit binary scientific data stored in raw raster or HDF files. NCSA Image produces color raster images according to user-defined palettes such as those created in NCSA PalEdit, or one of seven palettes built into the program. It also generates black-and-white contour, ordered dither, shaded data, and 3D plots. Using NCSA Image, you can plot linear selections of data in an XY graph, perform histogram equalizations on raster images, animate multiple raster images, and print any of the black-and-white plots. NCSA Image also allows you to rotate, compress, or expand colors within the active color palette and to view actual floating-point numbers.

NCSA PalEdit for the Color Macintosh Version 1.0
NCSA PalEdit allows you to interactively create customized color palettes. With NCSA PalEdit, you can modify individual entries in a palette or a palette as a whole to produce a palette tailored to best represent your various image data. NCSA PalEdit lets you save palettes in raw palette or HDF files, which can be read by NCSA imaging, analysis, and presentation tools such as NCSA Image, NCSA DataScope, and NCSA Layout.

NCSA Layout for the Color Macintosh Version 1.0
NCSA Layout helps you convey the results of your investigations and analyses to your colleagues in a professional form. It allows you to display and annotate 2D data images so that you can photograph your Macintosh screen display and generate 35mm presentation-quality slides. Your layout may include several images annotated with grid lines and tick marks, text, color bars that display the range of the current palette, and a colored canvas. By loading user-defined color palettes into NCSA Layout, you can vary the appearance of the images and the color of your text and canvas. You can save a layout as an HDF file that may be edited at a later date; or you can save any part of a layout as a raster image that may be transferred to other machines that support HDF for photographing, animation, or display.

NCSA HDF Specifications Version 2.0
NCSA HDF Specifications is a specification guide for developers who intend to build interfaces or utilities for HDF users. This guide is a supplement to be used in conjuction with the NCSA HDF software package.

How to download

If you are connected to Internet (NSFNET, ARPANET, MILNET, etc.) you can download software and documentation, and source code if it is available, at no charge from an anonymous file transfer protocol (FTP) server at NCSA. The procedures to do so are presented in the accompanying NCSA *Technical Resources Catalog Supplement*. If you have any questions regarding the connection or the procedure, consult your local system administration or network expert.

How to order

To order this software and any other software developed at NCSA, see the January 1989 issue of the *Technical Resources Catalog* or the accompanying supplement to this catalog. Order forms are in the publications. ▲

Call for software

by Scott Lathrop, Assistant Director, User Services

Please let NCSA know of any software needs so we may help provide you with the tools you need to do your research. Upon receiving a request for software, we will evaluate its cost, appropriateness for a Cray system, comparison of other available software, and support required. We will then let you know how we can respond to your needs. Please contact the software coordinators listed in the accompanying *Applications Software for the Cray Systems* for specific areas of need, or the Manager of Applications Software [see **NCSA Contacts,** page 23] for general assistance.

We are also interested in making software contributed by researchers available to the national community. If you have software that you would like to make accessible, please contact us.

To make software available, NCSA will need:

- abstract of the code
- statement of level of support available for software and consulting
- source code and steps to build an executable (this does not imply that the source will be made available to the community without your permission)
- documentation to be made available to other users
- newsletter article to describe the software and its purpose
- performance characteristics of the code on the CRAY

NCSA will evaluate the software to determine the level of support that NCSA can offer. This will vary from being unsupported and available on an as is basis to being fully supported. We will also periodically review the support level based upon usage and demand from users.

Please contact any of NCSA's software applications staff or the Manager of Applications Software to begin the process of making your code available. ▲

Academic Affiliates

Academic affiliates training—UNICOS

by Alan Craig, Manager, Training

Below. Academic affiliate training session.

NCSA hosted a training session January 6-10 for 27 representatives from 22 affiliate institutions. This was the first training for NCSA affiliates on the center's new UNICOS operating system. It was also a chance to bring these affiliate contacts up to date on what else is happening at NCSA.

Affiliate institutions and their representatives who attended the January training session are as follows:

Georgia Institute of Technology
Mary Trauner

Illinois State University
Richard Martin
Dean Sanders

Indiana University
Robert Holden

New Mexico Institute of Mining and Technology
Dave Becker
Jeff Garlough

Northwestern University
James Lindsay
Albert Lunde

Pennsylvania State University
Kevin M. Morooney

Southern Illinois University at Carbondale
Warren Snider

University of Arkansas
Bill Ashmore

University of California at Riverside
Paul Lowe

University of California at Santa Barbara
Stefan Boeriu

University of Chicago
Eric M. Nelson

University of Illinois at Chicago
Steve Roy

University of Iowa
Judy Brown
Gang Lu

University of Kansas
Ken Bishop
Michael Grobe

University of Missouri at Kansas City
Dennis McCormick

University of Missouri at Rolla
Terri Schierhoff

University of New Hampshire
Elizabeth A. Rivet

University of Notre Dame
Milind Saraph

University of Oklahoma
James M. Winters

University of Tulsa
Travis Tull

Vanderbilt University
Xin-Oi Yin

About training

NCSA conducts periodic training sessions for its academic affiliates. These training sessions are designed to help representatives from affiliate institutions become on-site consultants for their local researchers. Most representatives come from affiliates' campus computing centers, although several representatives are faculty researchers.

During the week-long training sessions, affiliate contacts are exposed to all facets of NCSA and meet the center's staff. The training sessions address technical topics, such as the center's CRAY X-MP and CRAY-2 systems, as well as the organization of the NCSA Academic Affiliates Program and the rights and responsibilities of affiliate campuses. Another benefit to participants is meeting representatives from other affiliate institutions. Training sessions are also a forum for affiliate representatives to voice opinions and concerns over the affiliates program and the services NCSA provides in general.

Program benefits

The NCSA Academic Affiliates Program brings supercomputing to campuses across the nation. Affiliate institutions receive a block grant of supercomputing time, special training, and other benefits. In exchange, each affiliate campus designates a person as the affiliate contact person to serve as a resource to NCSA users on their campus.

For more information about the NCSA Academic Affiliates Program, contact John Sfondilias [see **NCSA Contacts**, page 23]. ▲

Trainees respond

"Well-organized and well-presented; a very reasonable balance of topics."

"The overall training was most beneficial as an introduction to what is happening."

"Another well-organized, well-planned week."

"The whole week was very well presented. Many of the discussions were polished and done very well. Congrats."

"Fulfilled most expectations. Time and money was well spent. I now feel prepared to do battle in the trenches! . . . Thanks so much to everyone for their efforts."

John Sfondilias named academic affiliates coordinator

by Alan Craig, Manager, Training

A new face in the training group belongs to John Sfondilias (sfon DILL ee us). He is coordinating the NCSA Academic Affiliates Program.

Dr. Sfondilias comes to NCSA after working in Colorado as a private consultant to the US Air Force in satellite and space shuttle operations. Previously, he was at the Computer-based Education Research Laboratory (PLATO) at UIUC and at IBM as a systems engineer. Dr. Sfondilias received his Ph.D. from the UIUC in Instructional Design and Computer-based Education. His talents will be utilized to improve the training offered by NCSA.

The NCSA Academic Affiliates Program provides academic institutions with access to supercomputing resources, comprehensive training and support, and the opportunity to interact with over 70 other affiliate institutions. As coordinator of the program, Dr. Sfondilias says that his first priority "is to get to know the people involved at each affiliate campus, the research they are doing, and what their support needs are."

To learn more about the NCSA Academic Affiliates Program, contact John Sfondilias by telephone or electronic mail [see **NCSA Contacts**, page 23]. ▲

Above. John Sfondilias, coordinator of the Academic Affiliates Program.

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On the move

As the stacks of Macs in their new quarters show, some NCSA staff members are already moving over to the Beckman Institute. Among the first groups to move are the research scientists and the director and his staff. We will keep you posted in future issues of ***access***.

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Symposium continued from page 5

fraction of the cost of repeating the entire analysis for the new design. A videotape showed results from a design optimization developed by Dan Tortorelli, a recent UIUC Ph.D. graduate, with help from the Cray Applications Software Group. The design involved the transient thermal response of a metal casting design problem. The shape of the mold was modified during the optimization to shift the region of low-quality, high-porosity metal from the ingot region to the disposable riser region of the casting. In one sequence, the videotape showed an animation of the change in the temperature field (shown in color) as the design geometry was continuously varied.

Workstation demonstrations

In addition to the presentations, CRI provided space for workstation demonstrations. Dr. Wilhelmson, with the help of his research team, demonstrated the particle tracer code on the Stellar and NCSA Image [see ***access***, January–February 1989] and HyperCard animations on the Macintosh II. Dr. Haber demonstrated new software written by members of the NCSA RIVERS Group (Polly Baker, Steve Chall, and Ray Idaszak) for the Raster Technologies GX4000 graphics board set on a Sun-4/260 platform. The flexibility of the system was demonstrated through animations of crack data from Dr. Haber's research and cloud animations from Dr. Wilhelmson's work. ▲

data link Preview

Notes and quick tips

Finding the inside information on UNICOS
by Will Ridenour
Online Documentation Editor

UNICOS software applications update
by Beth Richardson, Applications Progammer, and Ilhan Dilber,
Industrial Consultant

CFT77 3.0 now available at NCSA
by Jim Ferguson
Industrial Consultant

Bidirectional memory on the CRAY X-MP under UNICOS
by Mark Straka
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EDA: Exploratory Data Analysis software installed
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by Michael Krogh
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Science

Supercomputer cancer research

by Kathleen Robinson, Science Writer

"I don't want to oversell ultrasound hyperthermia treatment as the ultimate way of treating cancer. Depending on the tumor type and position, there probably are a number of approaches that should be used synergistically." Charles Cain, UIUC professor of electrical and computer engineering and bioengineering, is discussing his current research into methods for treating cancer with the application of heat—hyperthermia. Dr. Cain and his colleagues in the Bioacoustics Laboratory design ultrasound phased array applicators for hyperthermia therapy, using computer models to optimize their equipment design. When he started this work in the early 1980s, Dr. Cain had to send his calculations to a supercomputer in Japan, but he now conducts his research using the NCSA CRAY X-MP/48 system.

Charles Cain in the Bioacoustics Laboratory with a 32-element phased array system.

Resurgent interest in hyperthermia

Hyperthermia cancer therapy is an experimental modality that is being investigated fairly extensively by a number of researchers. According to Dr. Cain, "Hyperthermia is not a new idea—people were interested in this at the turn of the century or even earlier. Several physicians experimented with bacterial toxins to cause fever, but I would say that the resurgent interest in hyperthermia is because of new techniques—particularly tissue culture—that allow biologists to investigate how heat can kill cells or interact with radiation to kill cells. It turns out that in the part of the cell cycle when cells are most resistant to radiation, they are quite sensitive to heat."

Clinical results

Hyperthermia cancer treatments depend on raising the temperature of a tumor to about 43°C for an hour or more. The difficulty is heating the tumor adequately without causing other damage. "Some tumors can be easily heated with available

Cancer research *continued on page 3*

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*Note: Italicized titles indicate boxed information. Since boxes are fillers, their subjects may not follow the topics of the heads under which they fall.

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Abbreviations

BI	Beckman Institute
CRI	Cray Research Inc.
IRC	Interdisciplinary Research Center of NCSA
NCSA	National Center for Supercomputing Applications
UIC	University of Illinois at Chicago
UIUC	University of Illinois at Urbana-Champaign

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***Cancer research** continued from page 1*

technology," says Dr. Cain. "Others can't—because of location, because of a peculiar shape, or because they happen to be highly perfused with blood." Increased blood flow, which counteracts the desired effect by cooling the tissue, is the body's response to the rise in temperature. To get an optimum temperature distribution requires a changing energy deposition during treatment. "This," says Dr. Cain, "is not a trivial thing to do."

Methods of heating tissue

There are several methods of heating tissue for cancer therapy. One technique is to use microwave energy, but this is not ideal for tumors deep in the body. When the microwave frequency is low enough for deep penetration, the wavelength is so long that heating is difficult to focus or control.

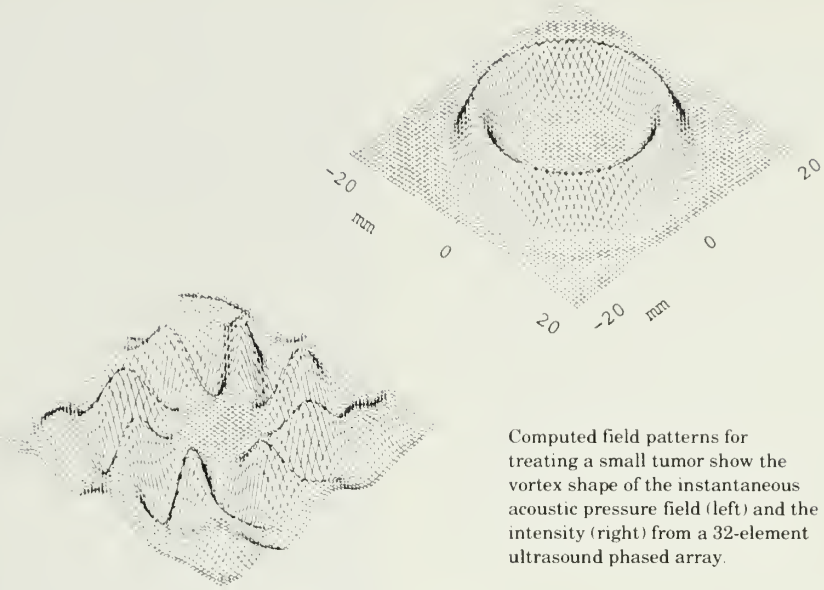
Another technique involves the use of ultrasound. One advantage of ultrasound is that frequencies which can penetrate deep inside the body have a relatively short wavelength that can be precisely controlled.

Ultrasound advantages

Fixed-focus ultrasound applicators produce a single small spot of focused energy that must be moved across the tumor tissue. Dr. Cain and others are working on more adaptable applicators that use phased arrays, which are multiple-element acoustic antennas. By adjusting the amplitude and phase of the signal which drives each element, they construct different patterns of energy deposition, so that the ultrasound treatment field can approximate the geometry of the tumor.

Another advantage of the phased array ultrasound applicators is that they produce a pattern that can be continuously varied in real time, allowing the operator to respond to temperature drops caused by increased blood flow.

"One of the technical difficulties that still needs a lot of research," explains Dr. Cain, "is getting appropriate temperature feedback from enough points. With ultrasound you can control energy deposition precisely, but currently there's no thermometry system available to allow clinicians to measure temperature with equal precision."



Computed field patterns for treating a small tumor show the vortex shape of the instantaneous acoustic pressure field (left) and the intensity (right) from a 32-element ultrasound phased array.

Anatomical model needed

Factors that affect the heat distribution in a tumor include the proximity of bone and air spaces. Says Dr. Cain, "Ultrasound doesn't propagate very well through bone, and it is almost totally reflected by any air space or gaseous inclusion in the body. And if bone is directly behind the treatment volume, there's a tendency for a hot spot to form at the bone-tissue interface. Eventually, we would like to use the supercomputer to simulate ultrasound hyperthermia treatment on an anatomically correct model of the body which allows for appropriate changes for all these variables."

Different geometries

Dr. Cain describes the phased array applicator as a two-dimensional surface of elements which are conformed differently depending on the intended use. "Each applicator that we design," he says, "has a different geometry and requires almost totally different programming. We built one applicator on a spherical shell. Another is fabricated on a section of a cylinder that surrounds the body. The geometry in each case is very different."

One possibility the group is considering is to construct the phased array on a flexible substrate so that each applicator would be appropriate for a variety of tumor locations. Explaining the limitations of such an approach, Dr. Cain says, "The range of tumor types and anatomical locations is rather large, so it would be difficult to design an applicator to fit every case. Applicators to heat superficial tumors, for example, would be operated at a different frequency and might require a different design than applicators used for other locations."

Role of the supercomputer

Phased array applicators are complicated devices and constructing prototypes is both time-consuming and expensive, so Dr. Cain and his group optimize all of the parameters in the design before building a prototype. "We use the supercomputer both to test our theory for phasing—by assuming a certain complicated structure with some number of elements having a particular geometry—and to compute the fields that would be produced in tissue. Then we use the results as input to a differential bioheat transfer equation, to compute the temperature for different blood levels. This gives us a

***Cancer research** continued on page 4*

***Cancer research** continued from page 3*

very good idea of how a device might perform in heating actual tissue with blood perfusion that changes with time."

In 1984, Dr. Cain started using supercomputers in his research while on sabbatical at the Hitachi Central Research Laboratory in Japan. He worked there with Dr. Shin-ichiro Umemura, an expert in the design of phased arrays for imaging. Says Dr. Cain, "It was very distressing to come back and realize that I couldn't do similar kinds of simulations in this country. Then NCSA was established, and it certainly made my job a lot easier. Before that, my choices were either to run 20-hour simulations on smaller computers here, or to send them to Japan."

"We write all our own software—it's not terribly complicated," Dr. Cain explained further. "In fact, I have all of my students write their own software, so they know what's going on. I find most students very reluctant to modify existing code. If something comes along that requires modification and they haven't already written software packages themselves, they are reluctant to make changes."

Experimental technique

When asked about hyperthermia cancer therapy's experimental status, Dr. Cain explains, "Before a modality becomes accepted in the clinic, there are a number of considerations. Of course, it has to be proven to be efficacious, which takes years. Clinical studies are currently underway. Then the economics of treatment is a consideration. I think hyperthermia is likely to be less expensive than some other techniques." Once again, he emphasized the role of a synergistic approach to cancer therapy involving combinations of treatment, such as hyperthermia and radiation, for optimum results.

Dr. Cain's research is supported by an NIH grant and some general funding from Hitachi, as well as the NSF support for NCSA, which he appreciates. ▲

Mike Norman reflects

by Kathleen Robinson, Science Writer

"What I do is computational astrophysics. I'm concerned with things depicted in coffee table books on astronomy—beautiful things like the Orion nebula." NCSA Research Scientist Mike Norman is, in fact, one of the pioneers who made possible some of the beautiful pictures we see in coffee table books, by combining simulations with scientific visualization to produce striking color images of computer models.

Radio galaxies, radio jets, and protostars

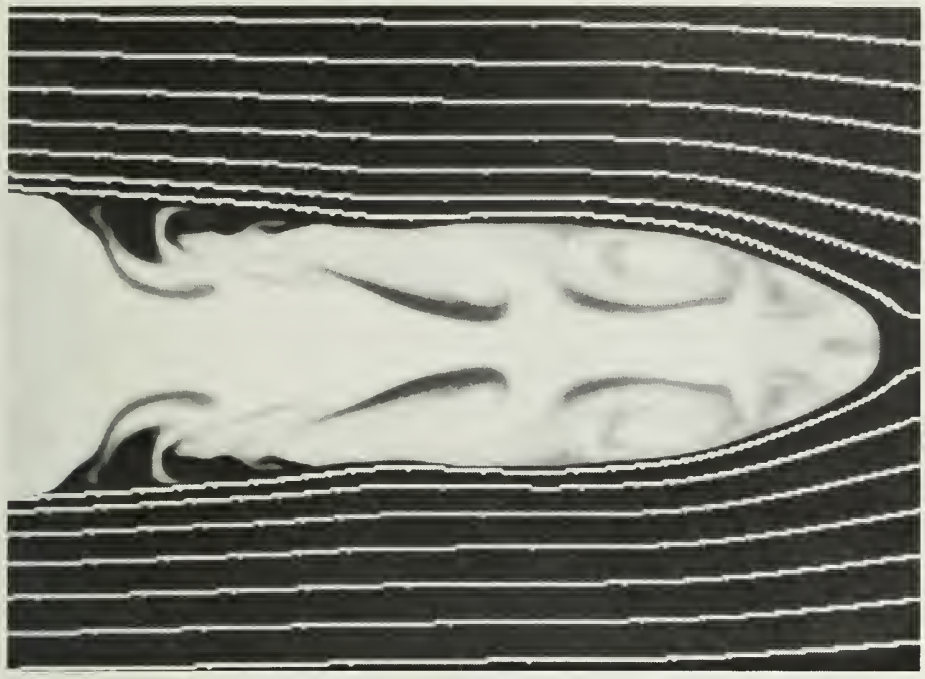
Dr. Norman has spent much of his time studying the origin and evolution of radio galaxies and their associated radio jets, though his initial interest was star formation. "That's the other branch of my studies—the dynamics of the ionized gas, plasma, that pervades space. Dense, interstellar clouds of plasma are the sites of new star formation—of protostars. *How* stars form is not exactly known, but the process involves gravity, pressure, centrifugal force, and finally—and this is something that has become accepted in the last 10 years—magnetic forces. I'm interested in the star formation process, in supernova remnants, in stellar winds—and how these interact in the interstellar medium."

Incorporating realistic thermodynamic descriptions of the plasma, Dr. Norman solves equations of magnetohydrodynamics (MHD). "What's beautiful," he says, "is that radio jets and protostars can be described by the same set of equations. Giant elliptical galaxies which produce radio jets are hundreds of thousands of light years in size, and the jets themselves range up to a million light years in length. Protostars are much less than one light *week* in diameter and have correspondingly smaller jets, yet the fundamental physics for generating the jets seems to be the same in both cases."

California collaborating

In 1976, Dr. Norman was a graduate student at "Teller Tech"—the Department of Applied Sciences of the University of California, Davis, located at the Lawrence Livermore National Laboratory. While there, he met Larry Smarr (at the time a recent PhD, now director of NCSA). Dr. Smarr had started some theore-

Mike Norman, research scientist.



A recent simulation using the ZEUS 2D code that shows the magnetic collimation of a protostellar jet. The calculation is performed in cylindrical coordinates, with the rotation axis lying along the x-axis. White lines represent magnetic field lines; shades of grey denote gas density where white is high and black is low. (Credit: Contour overlay using NCSA CompositeTool by Mark Stupar; simulation by Mike Norman and Jim Stone).

tical work on collapsing black holes, and had arranged to spend summers at Livermore to work on the numerical solution of the Einstein equations.

"We didn't interact too much at first—until 1979 when I was finishing my dissertation on star formation. Larry had just been visiting the astrophysicist Martin Rees at the Institute for Astronomy at Cambridge, England. Dr. Rees is one of the pioneers in the field of numerical astrophysics."

Dr. Norman remembers the infectious enthusiasm that drew him away from his dissertation writing and onto an unanticipated course. "Larry was then, as now, exuberant—full of ideas and worlds to conquer. He got me interested in modeling extragalactic jets. I had written a numerical code for my star formation study that could be applied to the jet problem. We collaborated on that, beginning six months before I got my Ph.D. He interrupted my writing, in fact. Then I went to Germany, to the Max Planck Institute for Astrophysics as a post doc with Karl-Heinz Winkler, who was also working on star formation in those days." Dr. Winkler, a member of NCSA's advisory board, is now director of the Numerical Laboratory at Los Alamos National Laboratory.

In October of 1980, Dr. Norman arrived at the Max Planck Institute in Munich, where he had access to a newly installed CRAY 1A supercomputer. It had "*one million words* of central memory," Dr. Norman remembers with some amusement. "A million words of memory was—you just couldn't imagine it. It was uncharted territory. We couldn't begin to use it, especially in astrophysics, where 20 by 20 grids—400 zones—were typical. In the summer of 1981 we used a staggering 50,000 zones. These days, people do simulations involving a million zones on NCSA's CRAY X-MP/48 system. But back then, 50,000 was a quantum leap."

Zones are small regions of space used to subdivide the problem domain; each zone is characterized by a set of state variables—density, pressure, velocity—which describe the local state of the fluid. The governing differential equations of fluid dynamics are then expressed as finite difference equations within these zones, which are then solved to advance the state of the fluid.

The CRAY 1A system allowed Drs. Norman, Smarr, and Winkler to construct the most detailed hydrodynamic model of an extragalactic jet that had ever been computed. The work was embraced by Martin Rees and the rest of the astrophysical community; it inaugurated an era of jet simulations. There are now a number of computational astronomers doing jet simulations, but the paper written in Munich after that summer's research was the first to show the detailed structure of jets.

After four years at Max Planck, Dr. Norman returned to work in the United States. "When I returned in the fall of 1984, there was no place for a computational junkie like myself to go. The national labs had the only supercomputers. So I took a position at Los Alamos doing research on relativistic particle beams. Actually, extragalactic jets are relativistic particle beams, so I was able to pursue my own research as well."

Arrival at NCSA

In February of 1986, Dr. Norman accepted a position at NCSA and has been at NCSA since that time, pursuing his research in astrophysics and directing the Computational Science Program since the fall of 1987. He recently passed the latter responsibility to Dr. Barbara Mihalas.

Dr. Norman is looking forward to the prospect of having more time to spend on his research. "We've just recently reached the point where we can make direct comparisons between our model and observed data. Hundreds of radio galaxies have been observed at high resolution with the Very Large Array radio telescope in Socorro, New Mexico, and radio astronomers have been able to draw some generalizations from this sample: the distribution of brightness in radio lodes, the distribution of polarization, and the spectral index (which relates to the state of the plasma that's producing the radiation). We captured those general features in an idealized simulation, though it was limited to a two-dimensional model."

Coding magnetohydrodynamics

NCSA Postdoctoral Researcher David Clarke is developing a 3D MHD code, continuing the project he began as a graduate student under Dr.

Norman *continued on page 28*

Renaissance Experimental Laboratory dedicated

by Kathleen Robinson, Science Writer

On April 21, James Clark, founder and chairman of Silicon Graphics, Inc. (SGI), formally dedicated the new Renaissance Experimental Laboratory (REL) located in the Beckman Institute. A large reception was held in his honor at the BI on the evening of April 20. Silicon Graphics IRIS Super System personal workstations are used by scientists, engineers, and creative professionals to design, analyze, simulate, and manufacture a wide array of three-dimensional products and services. SGI donated twenty IRIS workstations to NCSA, to create the REL.

Jim Clark (left) receives a plaque from NCSA Director Larry Smarr (right) at the dedication of REL.

Creating a new industry

SGI is a young company (incorporated in 1981), and the unprecedentedly large donation—worth $640,000—shows great faith in NCSA as a national training center for future computer graphics professionals. The donation "represents Silicon Graphics' commitment to education and research," says Mr. Clark. "As a leader in technology, Silicon Graphics is proud to support the model for the future that the Renaissance Educational Lab provides." NCSA Director Larry Smarr echoes that statement when he says, "This laboratory is a critical step toward our goal of educating a new generation of researchers. NCSA's joint efforts with SGI ensure that advanced computer technologies will be at the heart of tomorrow's curriculum."

Jim Bottum, NCSA deputy director, gives the donation a personal perspective when he adds, "It's very exciting to go into the REL and see all those students working on scientific visualization, when only two years ago we had to scour the world, seemingly, to find people to do this vital work. You might say we're creating a new industry."

REL is state-of-the-art

The purpose of the Renaissance Experimental Lab is to provide state-of-the-art computer graphics equipment for the development of interdisciplinary (thus, *Renaissance*) computer graphics courses that focus on scientific visualization and computational science.

Professor Donna Cox—principal investigator, REL director, and project leader—organized the first classes for the lab, which include computer science, mathematics, computational chemistry, biophysics, and art/design (see the sidebar on the opposite page). "Policies are being developed to ensure the widest possible use of this fantastic resource," she said, "that probably will involve the use of a peer review board for faculty who want to develop prototypical courses." Watch for policy statements and further information about using the REL in future issues of ***access***.

In addition to curricula development for universities, the lab will be used for scientific seminars and colloquia; plans are in place to use the REL as a teleclassroom to provide graphics instruction to scientists, professionals, and students in remote locations worldwide. This summer the REL will be available for use by NCSA researchers.

Mike Krogh, coordinator of REL and industrial consultant; Carl Hoyer, resource consultant; and Randy Butler, UNIX system administration, set up the lab.

IRIS workstation facilities

Each donated workstation is equipped with a 24-bit Z-buffer, 12.5 MHz floating-point coprocessor, 8Mbyte CPU memory, 170Mbyte internal disk drive, Ethernet, software developer's package, NFS, and C and Fortran compilers. Six cartridge tape drives were also donated.

The twenty cabinets that hold the CPUs of the IRIS Personal Workstations are purple, like the flowers with which they share a name. Standing upright beside keyboards and monitors, they give little hint of their power to unleash the imaginations of tomorrow's scientists and designers, or of the promise they hold for the future development of graphics education.

"Lots of great things are going to happen here," says Donna Cox confidently as she surveys the workstations. She is undoubtedly right. Some already have. ▲

Top Donna Cox teaches an art and design class in the REL.

Bottom Jim Clark of SGI (right) talks with Bob Wilhelmson, NCSA research scientist, (left) and Matt Arrott, NCSA scientific visualization specialist (center, back to camera).

George Francis on the REL:

"This spring is an experiment; we're running four classes in the REL," says **George Francis**, professor of mathematics.

"My class is a graduate mathematics class. In this course, students program the IRIS in C. For textbooks we used the *IRIS Programmer's Guide* and my *Topological Picturebook*. I prepared small programs and 'handed' them out electronically. So while I was lecturing, the students would be using them, looking at the code, and making the pictures move by moving the mouse. Then they had a chance to elaborate on the programs. Each program introduced new features as they went along. Halfway through, the students became independent.

"Running exclusively in the lab, **Donna Cox's** [assistant professor of art and design and research professor at NCSA] 300-level art and design course uses Wavefront software that was developed intimately with the IRIS. Even though it's very well adapted to the machine, it turns out to be difficult to teach. Donna is thinking of using different software in the future. It is called RT1 and was created by Tom Defanti [associate professor of chemistry, electrical engineering, and computer science] and Dan Sandin [professor of art and design] at UIC for electronic art and design.

"Students in **Scott Kahn's** [assistant professor of chemistry] chemistry course are expected to use QUANTA, CHARMm, MOPAC, and GAUSSIAN85 to visualize molecular models. Scott has been lecturing in his class on the subject matter, and the students use the software to visualize what he has been talking about.

"**Don Hearn's** [visiting professor of computer science] computer science course is an advanced course in computer graphics as applied to scientific visualization for graduate CS majors. He lectures, but his students do independent projects in the lab. Many of his students work with NCSA Research Scientists Bob Haber, Mike Norman, and Bob Wilhelmson.

"A fifth course, **Tony Croft's** [professor and chairman of biophysics] course in macromolecular structure through computer modeling is still in the planning stage. He hopes to be getting underway this summer." ▲

Cray R&D grant program presentations

by Mary Hoffman, Technical Editor

Below left Paul Saylor, UIUC professor of computer science.
Below right Arun Karalamagala, UIUC professor of electrical and computer engineering.

Above CRI representatives: (left to right) Kelly Altman, Tom Kemp, Jim Padian, and Eric Pitcher.

NCSA recipients of the 1988 Cray user research and development grants met at NCSA on March 16 to present summaries of their research projects. Representatives from Cray Research Inc. included Kelly Altman, account manager; Tom Kemp, region general manager; Jim Padian, region marketing support manager; and Eric Pitcher, director of university programs.

About the program

NCSA Research Scientist Mike Norman opened the meeting with a summary of the goals and scope of the program. The Cray Research and Development Grant Program encourages R&D projects which further the commercial or academic applications of Cray supercomputer systems by (1) significantly and uniquely increasing scientific, engineering, or computer system knowledge; or (2) developing software and/or algorithmic techniques for supercomputer architectures, thereby providing efficient or improved programming solutions to real-world problems. Cray grants have been awarded in the following disciplines: health sciences, physical sciences, biological sciences, mathematical and computational sciences, engineering, materials science, and microelectronics.

Scientific presentations

Dr. Norman briefly described the work of **Bob Haber** and **Stephen Lu**. Dr. Haber, associate professor of theoretical and applied mechanics and civil engineering at UIUC and adjunct associate professor at NCSA, has been a grant recipient since the program began three years ago. He has been pursuing computer simulation studies in crack propagation and is also well-known for visualization of the dynamic fracture of materials [see ***access,*** May–June 1988 and March–April 1989]. Dr. Lu, assistant professor of mechanical engineering at UIUC, has been performing metal forming simulations using NIKE2D code and optimizing it.

Dennis Cox, UIUC associate professor of statistics, presented for **Jerome Sacks**, professor and head of the department of statistics. Dr. Sacks' group has applied statistical methods to computer code used to simulate real processes by modeling the response as a random function (stochastic process) superimposed on a simple linear model. Using Best Linear Unbiased Predictors (BLUP), they can make probabilistic accuracy statements. In this way, they can model the whole function—not with just a crude approximation such as a quadratic polynomial—and, in the process, tune constants to observed data.

The methods employed by Dr. Sacks and his group have been applied to several concrete problems. In one such case, General Motors has been studying the process by which fiberglass Corvette auto bodies are

Below Michael Berry, CSRD computer scientist.

formed. Predictors have also been used with integrated circuits and methane combustion.

Optimizing the methodology

Michael Berry, computer scientist at the Center for Supercomputing Research and Development (CSRD) at UIUC, presented data on the Perfect Club Benchmark Suite, a collection of 13 public domain Fortran applications programs from air pollution modeling, computational fluid dynamics, seismic migration, quantum chromodynamics, and signal processing. The Perfect Club is a joint effort of universities, supercomputer companies, and research centers committed to (1) developing a methodology for creating a portable FORTRAN 77 benchmark suite of codes, (2) developing a methodology for measuring this suite, (3) producing effective measurements, and (4) identifying and categorizing code transformations needed for optimization. Most conventional benchmarking programs on the market do not offer correlated data or use kernels that are representative of a particular scientific workload.

Fundamental baseline measurements for the Perfect Suite include CPU time, wall-clock time, and Mflop rate. By keeping diaries on optimizing efforts, researchers can trace performance gains to compiler directives, software restructuring, and algorithm modifications. Once an optimal version has been produced on one machine, it can then be swapped around—thereby globally converging to a better benchmark, despite the specifics of each machine. The ideal machine would be able to maintain the increase across all codes.

Arun Karalamagala, professor of electrical and computer engineering at UIUC, spoke on "Algorithms for Signal and Image Reconstruction from Incomplete Data." From a small number of projections in lower dimensions over a limited angle, he and his group can faithfully reconstruct higher-dimensional objects, using sophisticated signal processing and some simple matrix manipulation techniques. Dr. Karalamagala has studied the results of three reconstruction algorithms: minimum energy extrapolation, autoregressive extrapolation, and rational extrapolation.

Minimum energy extrapolation is the method most often used, but it is sensitive to noise and errors in passband limits, and lacks the ability to resolve spectral peaks. The group has found that autoregressive extrapolation is excellent when peaks are sharp, but doesn't faithfully reproduce spectral plateaus. The rational extrapolation model, whose spectral estimate is the ratio of two FFTs, does well with both peaks and plateaus, but has the sensitivity problems of minimum energy reconstruction and is also sensitive to choice of model order. The group's current objective is to estimate model order from the rank of a matrix and to use singular value decomposition to achieve robustness.

Bob Wilhelmson, UIUC professor of atmospheric sciences and NCSA research scientist, is using a Cray supercomputer to produce a 13D storm model: 9 variables, 3 space, and 1 time. Dr. Wilhelmson wants to know (1) why some storm conditions engender tornadoes and others do not; and (2) how the curvature shown in hodograph data is related to the size of a storm. He has also been investigating low precipitation storms, which have a lot of rotation and reach a maximum updraft but grow relatively slowly (see ***access,*** September–October 1987 and March–April 1989).

Visualization has proved to be key in his study of storms. "What's driving the physical flow" is one of the questions that the project is trying to address with visualization. A 3D animation of a storm cloud with some 40,000 polygons, done with Wavefront Technologies Graphic Software, produces many of the tornadic elements but still does not rotate smoothly—even with very fast hardware. With Stellar and Cray supercomputer technologies, Dr. Wilhelmson has shown live trajectories with 500 particles. He plans to do this simulation with hundreds of particles in order to delineate the whole turbulent flow.

Millions of unknowns

Paul Saylor, UIUC professor of computer science, has been working on the "Iterative Solution of Large Sparse Matrices by Leapfrog Variants of Richardson's Method." The problem is to solve $Ax=b$ where A is large, sparse, and possibly complex. Experimental results for the leapfrog variant show tiny gains due to increased number of terms in vector sums. Further advantages include nested evaluation of matrix polynomials and reduced I/O traffic for large problems. One such "large problem," Dr. Saylor says, is to solve Maxwell's equation in three dimensions, which involves some 20 million unknowns.

John Nicholas, graduate student, presented for **Anton J. Hopfinger**, professor—both of the medicinal chemistry department at UIC. Hopfinger's group has been pursuing three projects on the Cray: (1) phase transition of polystyrene; (2) delimiting the structure of sulphonamides, important in agriculture as herbicide and antibacterial agents; and (3) molecular dynamics of zealites with argon, inorganic silicon, boron, and oxygen crystals. Zealites are valuable for industrial use as molecular sieves; for example, they can capture long-chain alcanes to yield high-octane gasoline.

***Presentations** continued on page 10*

Presentations continued from page 9

Dr. Hopfinger is studying ZSM5, a 300-atom zealite which has silicon at the junction and oxygen in between. He has discovered three diffusion paths for ZSM5: long, or stray channels where the molecule is unhindered; secondary, where they hit the junctions, and short paths where the molecule must zig-zag to get through. This experiment has been expanded with 100 methane molecules and shown to be in agreement with neutron diffraction techniques. Mr. Nicholas says the group will have a "truly huge calculation on our hands" in the next experiment when they add benzene with ZSM5—a full-scale production will require 20 Cray computer hours.

Bruce Mason, UIUC postdoctoral research associate at the Coordinated Science Laboratory, presented the results of **Karl Hess**, UIUC professor of electrical and computer engineering and principal investigator of the Semiconductor Physics Group [see ***access,*** September–October 1988]. Their theme is "From Physics to Function." By using first-principles physics and Monte Carlo methods, they are studying how electrons move through semiconductors. The more computationally intense the simulations become, the more they need the power of a Cray supercomputer—for example, including electron-electron or higher-order electron-phonon interactions.

Dr. Hess's group is also investigating quantum inference devices, and the electron transport properties of novel semiconductor structures, such as the heterostructure hot electron diode. Another major project is the modeling of ultrafast laser spectroscopy experiments. Graduate student **Dan Bailey** presented some of the results of this work by showing a videotape of the electron distribution in the first conduction band of GaAs after subpicosecond optical excitation. Mark Bajuk, NCSA scientific animator, constructed the graphics of the movie.

Expansion in 1989

The Cray Research and Development Grant Program for 1989 includes expansion in the following areas:

- dissemination of opportunity, including all University of Illinois departments and all NCSA Academic Affiliates;
- supercomputer architectures with the CRAY-2;
- computational opportunities through multiprocessing and distributed applications on UNICOS and interactive applications on the ULTRA Frame Buffer;
- participation on both Cray machines, with six new grants on the CRAY X-MP and nine new grants on the CRAY-2 supercomputer; and
- disciplinary coverage. ▲

Are you interested in working at NCSA?

by Marcia Miller, Manager, NCSA Administration

NCSA continues to grow and expand, so there are frequent openings for part-time and full-time staff. We want to encourage anyone interested in working at NCSA to submit a résumé, even before positions may actually be opened. When a position is created and a formal search has begun, we will contact those of you who have submitted résumés that fulfill the requirements of the position. After you receive this notification, you may then formally apply for the particular position, in accordance with the hiring procedures of UIUC.

We continue to advertise all open positions according to UIUC regulations, but having résumés already on file helps us identify people with appropriate backgrounds who may be interested in applying for a position at NCSA.

In addition, we post open positions on the front-end VAX NOTES under the conference named NCSA_JOBS. This allows NCSA users to log on and check on open positions at their own convenience.

We would like to receive résumés from people with advanced degrees in various scientific disciplines (including engineering, chemistry, and mathematics) and with experience in any or all of the following areas:

- supercomputing experience with large-scale systems such as Cray computers
- parallel processing
- visualization and graphics
- UNIX
- user support (consulting, training, documentation)

Send your résumé to Marcia Miller, NCSA Administration, 152 Computing Applications Building, 605 East Springfield Avenue, Champaign, IL 61820.

NCSA is an affirmative action/equal opportunity employer.

NCSA mass storage system upgrade

by Curt Canada,
Mass Storage Systems Programmer

To deal with the increased mass storage requirements of the NCSA computing complex and to position NCSA for future requirements, the mass storage system hardware was upgraded on April 1—converting from an IBM 4341-P2 processor to an Amdahl 5860 processor, increasing disk from 12.5 to 60 Gbytes, and tripling the cartridge tape capacity to 3 channels and 12 transports. This upgrade immediately increased both the amount of storage available and the speed at which files are transferred for the user. During 1989, an additional 60 Gbytes of disk will be added as needed to meet storage demands.

This mass storage upgrade results from the efforts of several staff members to establish a new strategic partnership with the Amdahl Corporation. Not only has NCSA purchased the mass storage system at a favorable price, but NCSA will also share in evolving technologies in partnership with Amdahl, the National Aerodynamics Simulator Facility at the NASA/Ames Research Center, and other Amdahl customers.

Fast, reliable access by researchers to their files is essential for effective use of a supercomputer. NCSA's mass storage system achieves this through use of the network-based hierarchical Common File System (CFS) software developed at Los Alamos National Laboratory (LANL) and enhanced at NCSA. CFS and its companion MASS/CFS utilities on the CRAY X-MP and CRAY-2 systems and VAX front ends provide NCSA researchers with access to highly reliable and cost-effective storage devices for long-term file storage.

Curt Canada, mass storage systems programmer, at the console of the Amdahl 5860 with disk storage farm to the left.

Storage management

CFS manages files in a two-level hierarchy of increasing access time and capacity, and decreasing cost. The two levels are Amdahl 6380E disk and StorageTek 4480 tape. By migrating files automatically between the levels based on their activity and size, performance comparable to a disk-only storage system can be achieved at a fraction of the cost. CFS uses the high-performance disk in a manner analogous to the high-speed memory cache of large mainframes. As files arrive (i.e., when a user saves or replaces a file with MASS/CFS), CFS selects a storage device based on the size of the file, placing files greater than 8 Mbytes on tape and smaller files on one of three categories of disk. Special provisions are available for storing large numbers of small files directly on tape instead of disk when appropriate (e.g., tens or hundreds of images, each less than 8 megabytes). On a daily basis, files are selected for migration between disk and tape using a *space-time working set* algorithm developed by Duncan Lawrie and Mike Randall at UIUC after a three-year study of user file activity on its 10,000-user CDC system. The algorithm has proven itself in the NCSA environment by maintaining an 85% disk hit ratio for user requests during the first few months of 1989 with a very limited disk capacity. One of the most apparent effects of the hardware upgrade is the increase in disk capacity to 60 Gbytes which has raised the disk hit ratio to approximately 95%.

Amdahl 5860 processor

The Amdahl 5860 is a System/370 compatible scalar uniprocessor with 64 Mbytes of memory and 32 channels (twenty-four at 3.0 Mbytes per second and eight at 4.5 Mbytes per second.) The 5860 is field upgradable to a 5880, with two tightly coupled processors—twice the memory and twice the channel capacity of the 5860. The 5860 processor is air-cooled ECL technology and is about ten times faster than the previous mass storage system processor, the IBM 4341-P2. These increases in capacity have resulted in significantly higher data transmission rates, which now peak at 1.2 megabytes per second. The peak rate with the 4341-P2 was 600 Kbytes per second.

Upgrade *continued on page 12*

Upgrade continued from page 12

By using the Multiple Domain Facility or MDF, the 5860 is capable of running up to four operating systems simultaneously—each in its own completely independent domain. Currently, the only production domain is one for CFS. In the future, one or more domains will be activated to begin research and development with Amdahl's UTS operating system, which is based on AT&T's UNIX System V. ▲

Consulting assistance

by Dave McWilliams, Manager, Consulting

NCSA's consulting staff is here to help users make the most efficient and effective use of the various facilities and services offered by NCSA.

When you need technical assistance or information, the first place to turn is the Consulting Office.

You may reach the office by calling (217) 244-1144, by sending electronic mail to consult@ncsavms (BITNET), or by walking into room 54 of the Computing Applications Building. To provide a prompt response to our remote users, our first priority is to assist people calling in by telephone. The office is open from 8 a.m. to 5 p.m. CST, Mondays through Fridays. At other times, an answering machine records messages.

The Consulting Office is staffed primarily with 8 graduate students and 1 undergraduate student. In our process of selecting graduate students, we have been quite fortunate in hiring a number of people that have prior experience working on the NCSA Cray systems as part of their own research efforts. Having graduate students that are using the system for their own research provides you with support by people that are using many of the same tools and techniques you are using as well as people that understand many of the problems and issues you face. Our current graduate students are now working in these fields: electrical engineering, computer science, mathematics, mechanical engineering, and physics.

By having students staff the Consulting Office, the full-time consultants have been able to focus on supporting users with difficult questions concerning vectorization, optimization, multitasking, graphics, and general debugging analysis—to name a few areas. The consultants and the applications staff also provide in-depth support in the selection and usage of the software libraries and packages available on the systems. The full-time consultants are also able to focus on the support of researchers that come to NCSA through the Visitors Program. Each of the student consultants is assigned to work with a full-time consultant or applications staff member to become actively involved in software projects on the Cray and to further develop their own specialties.

If a problem raised by a researcher gets quite involved, we will often also call upon one of the staff research scientists to assist in understanding and resolving a question. Our research scientists cover the following fields: quantum statistical mechanics, quantum gravity, radiation transport, fluid dynamics, numerical relativity, symbolic manipulation, quantum chemistry, and atmospheric sciences.

NCSA's goal is to provide users with a point of contact for quick answers to common problems and referrals to other staff experts for more difficult or involved questions. As in all other aspects of NCSA, we welcome your comments about the effectiveness of NCSA's consulting support. We also welcome suggestions for improvement. Please feel free to contact Dave McWilliams, the manager of Consulting, or Scott Lathrop, assistant director of User Services, with your comments and suggestions [see **NCSA Contacts,** page 27]. ▲

UNICOS migration

by Scott Lathrop, Assistant Director, User Services

The migration from CTSS to UNICOS is now complete, but NCSA's work is far from done. NCSA will continue to work to improve the UNICOS environment with additional tools, utilities, and applications software. Toward this end, NCSA needs your comments and suggestions for ways in which it can improve the environment and enhance the software available on the system.

The next major effort will be to upgrade from UNICOS 4.0 to UNICOS 5.0, which we expect to do by this summer. We will keep you informed of the plans for these changes and the possible impact upon usage of the systems. The major enhancements to be found in UNICOS 5.0 include:

- fair share scheduler
- more compatibility between the CRAY-2 and CRAY X-MP systems
- full support for BSD 4.3 TCP/IP, including Berkeley sockets and line printer spooling
- autotasking and improved vectorization available on both Cray systems
- Fortran profiling improved

NCSA wishes to express its appreciation to all users for the many recommendations and suggestions. Please continue to let us know how we can improve things for you. ▲

Allocations on the supercomputers

by Patricia Wenzel, Manager, User Administration

NCSA has time available to allocate on the supercomputers. Researchers are encouraged to submit applications for time on the CRAY X/MP-48 system, the CRAY-2 system, or both systems.

Applications for 100 or more service units (SUs) will be reviewed at the next Peer Review Board (PRB) meeting in September (August 1 application deadline). Applications for fewer than 100 SUs will be sent out for external review and allocated by the Small Allocation Committee, which meets monthly.

The PRB meets quarterly to review applications for allocation. Application deadlines remain the same from year-to-year, and they are as follows:

Application Deadlines	**PRB Meetings**
August 1	September
November 1	December
February 1	March
May 1	June

UIUC dedicates Beckman Institute

by Fran Bond, Technical Editor

Touring NCSA's facilities in the Beckman Institute during the dedication activities are: (left to right) Ted Brown, director of the Beckman Institute; Larry Smarr, director of NCSA; Gerald M. Edelman, Nobel Laureate in Physiology and Medicine from Rockefeller University; and George Francis, professor of mathematics at UIUC.

The Arnold O. and Mabel M. Beckman Institute for Advanced Science and Technology, thought to be the largest and most broadly based interdisciplinary research center anywhere in the world, was officially dedicated this spring. The 300,000-square-foot building designed by Detroit architects Smith, Hinchman, & Grylls Associates Inc. [see ***access,*** July–August 1988], is the site of NCSA's scientific research program, R&D in advanced technologies, national visitors program, and director's staff. In addition, the Beckman Institute is headquarters for approximately 20 UIUC interdisciplinary research programs. In a recent speech to the NCSA staff, Director Larry Smarr said that being situated in the BI is "an unparalleled opportunity" for NCSA's growth.

Dr. Gerald M. Edelman (*see left*), 1972 Nobel Laureate in Physiology and Medicine and director of the Neurosciences Institute at Rockefeller University in New York City, gave the inaugural address entitled "Neurobiology and the Coming Scientific Revolution."

As part of the activities of the inauguration, NCSA displayed and demonstrated software applications developed by the Software Development Group (SDG). The newly established Renaissance Experimental Laboratory (REL) was open to the public, also. Visitors to both exhibits had the opportunity for hands-on time.

Constructed on the site of UIUC's first building, the BI was funded by UIUC alumni Mr. and Mrs. Beckman for interdisciplinary research. Their $40 million gift is thought to be the largest individual donation to a public university. ▲

Nora Sabelli, research scientist, joins NCSA

by Fran Bond, Technical Editor

Nora Sabelli, senior research scientist.

Dr. Nora Sabelli joined NCSA as a senior research scientist February 1. Concurrently, Dr. Sabelli will retain her membership on the faculty at the University of Illinois at Chicago (UIC) where she is an associate professor of chemistry. She specializes in quantum chemistry ab initio methods, and at UIC, she teaches advanced courses in chemistry. She is also a member of the Computational Chemistry Group headed by Dr. Harrell Sellers, research scientist.

Last academic year she developed an innovative Graduate Student Workshop Program on Scientific Supercomputing using NCSA's CRAY X-MP/48 system [see ***access***, May–June 1988]. As part of the workshop curriculum, UIC students visited NCSA to utilize the Cray supercomputer, so Dr. Sabelli is no stranger to the IRC.

"Nora has been helping NCSA for at least the two and one-half years that I have been at the center," says Deputy Director Jim Bottum. "Her work in supercomputing education is state-of-the-art. As one of our industrial partners said when I told him we had a chance to get Nora at NCSA, 'That would be a stroke of genius!' It was. NCSA is very fortunate to have Nora on staff."

At NCSA, Dr. Sabelli's role is to carry out research, give guidance to the training program, and develop educational programs in computational science whereby UIUC and NCSA work with other universities. Her primary educational interests are in using supercomputers to teach scientific concepts. Her educational efforts will be addressed not only to graduate students but to professionals and undergraduates as well. Dr. Sabelli's research focus is in unstable negative resonances, and she works in an area that interfaces chemistry with physics. While at NCSA, she has been collaborating with scientists at Argonne National Laboratory on quantum trajectory codes. Her work in training and education will be in association with Alan Craig, manager of Training, and Scott Lathrop, assistant director of User Services.

Plans are already underway for a Summer Workshop on Supercomputer Education at the Beckman Institute and the Computing Applications Building from July 10 to 21 [see ***access***, March–April 1989]. This workshop is directed to those who use supercomputers and want to educate others about them. Oriented toward the concepts of computer science that are basic or necessary to computational science, lecturers will come from other supercomputer centers and universities.

Currently Dr. Sabelli is developing a demonstration course to be offered next academic year, probably in the spring semester. Designed to introduce computational science concepts into the classroom, this class is for graduate students and some undergraduates. A modular concept is planned for the course which utilizes an interdisciplinary approach. This course is partial fulfillment of one of Dr. Sabelli's goals for NCSA: to develop modular courses and course materials that faculty can adapt to their own needs.

Dr. Sabelli's other objectives include:

- making joint proposals to NSF and private foundations together with outside universities and colleges in exchange for information and publications;
- developing software interfaces, in collaboration with NCSA's Software Development Group, to reduce or eliminate the time needed to introduce the use of supercomputers in applied courses; and
- proselytizing and publicizing successful projects to increase the visibility of NCSA.

Dr. Sabelli learned how to use computers and to respect them as valuable research tools while doing graduate work at the University of Chicago. At that time, she says, "networking" consisted of making phone calls between Bell Labs in New Jersey and her lab at the university. "I learned everything I know about computers by hitting my head against a wall, and I don't see why anyone else should go through the same thing now," she says. Indeed, this comment encapsulates her philosophy of supercomputing education.

A native of Argentina, Dr. Sabelli earned her Ph.D. in chemistry from the University of Buenos Aires while carrying out her research at the University of Chicago. After getting her doctorate, she went back to Argentina to teach at the University of Buenos Aires and the University of Litoral. Later she returned to Chicago to teach at UIC. She was coordinator of Large-Scale Computing at the Computer Center while at UIC. ▲

Ecological researchers at NCSA

by Kathleen Robinson, Science Writer

A wide-area conference and workshop for NSF Long-Term Ecological Researchers (LTER) was held at NCSA April 26–28. Seventeen sites were represented, with participants from as far away as Alaska and Puerto Rico. Lectures, a panel discussion, and lab sessions with hands-on experience comprised the workshop. Participants also got to try out the CRAY X-MP/48 system.

Early in the sessions, Dr. Tom Callahan of NSF's Biological, Behavioral, and Social Sciences Division, said, "The reason for this workshop is to make the LTER network a reality." He explained that although the first LTER awards were made in 1981, only recently have most of the sites had network access. NSFNET and Internet access gives LTER researchers—who are often at sites that are truly "remote"—the means for data transfer, access to resources, and the possibility of collaborating with other researchers. He mentioned two advantages that network access to supercomputers gives to environmental research: fast computational speed—necessary for ecological modeling, and parallel processing capabilities. "Ecosystems themselves are large parallel processors," Dr. Callahan said, "so it's time to take advantage of that fact and use the architecture that's becoming available."

Making an analogy to a 19th-century machine shop with its innovative central power source that today seems antiquated, Bob Robbins, also of NSF's Biological, Behavioral, and Social Sciences Division, said, "We're still in the quaint stage of networking at this point. Connectivity is the trick. We want the network system to be as good as the mail service or the telephone."

Participants were introduced to a wide array of network resources. Many of the LTER sites already use electronic mail facilities, but researchers may not have been aware of the many relevant bulletin boards and other resources that were introduced.

Karen Roubicek of BBN Systems and Technologies Corporation, the NSFNET Service Center (NNSC), said that directories of people and resources are in great demand. She described the program WHOIS, which provides the names and addresses of thousands of researchers worldwide. That program is maintained at the Network Information Center, but many systems can run WHOIS locally. She also gave participants the electronic addresses of several libraries. Explaining that these libraries usually list books, rather than journal articles, she noted that users can search by topic and also can request lists of the most recent acquisitions.

Participants left the conference with stacks of information and increased confidence in using the network resource. Besides practice with electronic networking, there was a great deal of personal "networking." For further information, contact Alan Craig, manager of Training, who organized the workshop [see ***NCSA Contacts***, page 27]. ▲

LTER workshop.

Selected upcoming meetings in 1989

NCSA 1989 Summer Institute
June 19–30
NCSA, Computing Applications Building, Champaign, IL
For more information, contact Alan Craig, manager of training, at (217) 244-1988

NCSA Summer Workshop on Supercomputer Education
July 10–21
NCSA, Computing Applications Building, Champaign, IL
For more information, contact Nora Sabelli, workshop coordinator, at (217) 244-0644 or nsabelli@ncsa.uiuc.edu

Massively Parallel Computing Summer Workshop
July 31–August 4
NCSA, Computing Applications Building, Champaign, IL
For more information, contact Michael Welge, workshop coordinator, at (217) 244-1999

13th Conference on the Numerical Simulation of Plasmas
September 17–20
Hilton Hotel, Santa Fe, NM
For more information, contact Mike Norman, member of Scientific Organizing Committee, at (217) 244-2006

NCSA User Group Meeting
October 23–24
NCSA, Beckman Institute, Urbana, IL
For more information, contact Janice Knapp-Cordes, assistant training coordinator, at (217) 333-0085

Daniel Alpert, special consultant to NCSA

by Fran Bond, Technical Editor

Daniel Alpert, special consultant.

Recently Daniel Alpert became special consultant to the director of NCSA. He will also be working closely with the deputy director and the chair of the research scientists group to develop policies and practices for NCSA's interdisciplinary thrusts.

"Dan Alpert 'wrote the book' on interdisciplinary research organizations. He is coming to NCSA at a critical time in our evolution," says Deputy Director Jim Bottum, in reference to NCSA's recent expansion into the Beckman Institute.

Dr. Alpert's role is to encourage and strengthen NCSA's capacity for contributing to the BI, to the UIUC campus, and to the national scientific community which NCSA serves.

Not only does Dr. Alpert bring extensive experience in administration and development of interdisciplinary research organizations, he is published widely on the issues and challenges of such centers also. "Performance and Paralysis: The Organizational Context of the American Research University," is the intriguing title of his influential paper published recently in *The Journal of Higher Education*. In this paper, he points out the need for a new type of interdisciplinary research organization, or IRO, that is motivated to advance important scientific fields by offering "multiple perceptions," "integrative approaches," and "alternatives to [traditional] reductionist approaches"—especially in the physical sciences—through "new settings, new groupings of faculty, and new incentives" which are not available in the existing academic structure. In a later paper, Dr. Alpert cites NCSA as a distinctive example of the new IRO as he defines it.

Aside from his administrative expertise, Dr. Alpert has a distinguished record as a research physicist and technological innovator. After receiving a Ph.D. in Physics from Stanford University, Dr. Alpert joined Westinghouse Research Laboratories in 1941. During World War II, he participated in the development of components used in radar systems for the military and in the Manhattan Project. After the war, he returned to Westinghouse to do basic research and became manager of the Physics Department. In 1980, he received the Gaede-Langmuir prize of the American Vacuum Society for his work at Westinghouse in the development of ultrahigh vacuum technology—now widely used in scientific instruments, particle accelerators, and advanced materials processing.

In 1957, Dr. Alpert joined the UIUC faculty as professor of physics and technical director of the Control Systems Laboratory which he later reorganized, directed, and renamed the Coordinated Science Laboratory (CSL). At CSL he developed an interdepartmental, problem-oriented program aimed at applying modern computer technology to significant public sector problems. In addition, he played a key role in the initiation of PLATO, the computer-based education program, and in its administration and development for 15 years.

Appointed dean of the UIUC Graduate College and chairman of the UIUC Research Board in 1964, he was instrumental in establishing several campus interdisciplinary and multidisciplinary organizations. Those founded under his leadership include: the Computer-based Education Research Laboratory (CERL), the Center for Advanced Computation (CAC), and the Computer Services Organization (CSO). CAC was set up to be the research organization built around the ILLIAC IV supercomputer.

In 1964 he was awarded a Guggenheim Fellowship to study the role of university professors in addressing problems posed by society. Four years later, he chaired a study, "The Impact of Science and Technology on Regional Economic Development," sponsored by the National Academy of Sciences and the National Academy of Engineering. A continuation of Dr. Alpert's interests in science and technology policy and the governance of academic R&D organizations led to his becoming director of the Center for Advanced Study (1972-87) and director of the UIUC Program in Science, Technology, and Society (1986-present).

In the immediate future, Dr. Alpert will develop and implement plans for an intellectual center within NCSA. On the one hand, it will provide opportunities for professional interaction and collaboration among the wide variety of programs within NCSA—including academic as well as industrial scientist-engineers. In addition, NCSA will identify and encourage the formation of multiple networks of collaborating faculty members, postdocs, visiting scholars, and graduate researchers—representing a wide variety of supercomputer applications. These networks, with NCSA as a key node or catalyst, will extend in many directions in the BI, the UIUC campus, and the national scientific and engineering communities.

Dr. Alpert's other responsibilities at NCSA will include:

- working with NCSA research scientists and adjunct faculty on administrative policies and practices for this level of professional participation; as well as building relationships with other key players in NCSA, BI, and UIUC, to develop an approach for setting scientific goals and advancement of state-of-the-art technology for science;
- providing administrative leadership for the development of educational projects that (1) will be characterized by the utilization of advanced computational and visualization technologies, (2) will address problems typified by those addressed in NCSA research, and (3) will include instruction in the use and applications of advanced computer-based technologies; and
- maintaining a broad range of communications to interrelate the efforts of NCSA personnel, BI faculty, and UIUC faculty and administrators.

"The way I see it," says Dr. Alpert, "NCSA offers an opportunity for the American research university to relate to itself in a new level of cross-disciplinary interaction—providing access to powerful new tools for almost every discipline, and ways of dealing with large-scale problems otherwise intractable. This is a tremendous challenge; NCSA runs crosswise—orthogonal to the way a university is organized—and could widen the existing gaps within the larger campus community. The opportunity is even greater: if done with care and sensitivity, NCSA's relationship to the larger university could be a source of great reward and symbiotic achievement." ▲

University Board of Trustees visit NCSA

When the University of Illinois Board of Trustees met recently at UIUC, they visited NCSA and its facilities. As part of the tour, they got an opportunity to inspect the CRAY-2 supercomputer along with President Stanley Ikenberry. Trustees are: (left to right) Nina Shepherd, Susan Gravenhorst, Charles Wolff, Judith Reese, student trustee Jim Evenson, Kenneth Boyle, and Glora Bacon, with President Ikenberry (Credit: Photo by The Champaign-Urbana News Gazette).

Scientific visitors

Andrew Abrahams.
April 8–13 from Cornell University.
Area of research: general relativity.

Giovanni Bachelet.
April 13–July 15 from University of Trento.
Area of research: physics.

Gilbert Mains.
April 17–20 from Oklahoma State University.
Area of research: chemistry.

Walid Abu-Sufah.
May 8–July 8 from Virginia Polytechnic Institute.
Area of research: computer science.

Ed Seidel.
April 8–13 from Washington University.
Area of research: general relativity.

Paul J. Wiita.
April 16–22 from Georgia State University.
Area of research: astrophysics.

Harold Alden Williams.
April 15–May 12 from Carnegie Institution of Washington.
Area of research: astrophysics.

NCSA cosponsors Parkland computer graphics program

by Jarrett S. Cohen, Student Technical Editor

The field of computer visualization received a boost recently in the form of a new program at Parkland Community College in Champaign. Entitled "Advanced Certification Program for Visualization Computer Graphics Specialists," it will train students to become visualization programmers. In this effort, NCSA and BI are collaborating with Parkland to teach computer visualization.

Citing a University of Alaska School of Management study, an editorial in a recent issue of *Computer Graphics World* stated that "the number one obstacle to the increased use of computer graphics is insufficient user knowledge." People involved with the Parkland program agree with this assessment. "There is a great lack of trained technicians to do visualization work, and those that are capable are largely self-taught," says Parkland Program Director Sunny Christensen. "Scientific visualization is a field that is pioneering an entirely new, advanced form of communication."

The program will teach students to think visually and then make computerized visual representations of scientific data generated by supercomputer applications in support of research. Michael Krogh, NCSA industrial consultant and an instructor in the program, says, "Other schools have graphics programs, but they are more for graphics research. Ours is mainly a vocational program."

Embedding diagram of a black hole obtained from a numerical solution of the Einstein equations that describe the gravitational field; background is the Cygnus region (Credit: "Numerical Relativity Black Hole Space Times" by Larry Smarr, David Hobill, and David Bernstein—research scientists; Donna Cox and Ray Idaszak—visualization).

Funding

The program is funded through a $235,000 grant from the U.S. Department of Education. Mrs. Christensen wrote the program proposal, which was ranked ninth out of 37 applications for new projects. In the high-technology category, "our proposal was chosen as an example of quality proposal writing," she says.

Mrs. Christensen attributes the obtaining of the grant to the involvement of NCSA and a generous donation of equipment to NCSA by Silicon Graphics, Inc. NCSA staff who developed the grant include Mr. Krogh; Scott Lathrop, assistant director of User Services; Donna Cox, assistant professor in the UIUC School of Art and Design and research professor at NCSA; and Ray Idaszak, visualization research programmer and software/hardware technical lead for the classroom. Mr. Idaszak is also an instructor in the program.

Silicon Graphics, Inc., headquartered in Mountain View, CA, donated 20 IRIS Personal Super Systems, worth an estimated $35,000 each, to NCSA. The IRIS workstations are in the Renaissance Educational Laboratory (REL) at the Beckman Institute, part of the Renaissance Team Educational Project. Professor Cox is the principal investigator on the SGI grant and the project leader for the Renaissance Experimental Laboratory and Educational Project. (See page 6 of this issue of ***access*** for the details.) Students in the visualization program will use these machines for their classwork and during their internship training.

First of its kind

This program is the first of its kind in the United States. The idea for the program first came up one and one-half years ago, when Dr. Paul Magelli became the president of Parkland, says Mrs. Christensen. Meetings with NCSA Director Larry Smarr have resulted in a number of collaborations, including one with the school's Staerkel Planetarium [see ***access***, May–June 1988].

Dr. Magelli points to the usefulness of collaborating on this project. "The computer graphics specialist training program, which brings together the technological resources of NCSA and the educational expertise of Parkland College, holds tremendous promise for developing new career opportunities for students," he says. NCSA will benefit in that it "will help us expand our own training program in graphics and visualization," adds Mr. Lathrop.

Entrance requirements and curriculum

Requirements to enter the program include a knowledge of math through college calculus and basic computer literacy. For those students who need a refresher course in mathematics, a review of calculus is being offered this summer. In addition, there is a class in the C programming language. The summer classes and the bulk of the fall and spring curricula are being taught at Parkland.

Fall offerings

The fall offerings include classes in C, Fortran, the UNIX operating system, and illustration. The illustration class will focus on design, color, and pattern. The main course of the semester is Computer Graphics I. "Computer Graphics I is a fundamental course which will give students experience with two- and three-dimensional computer graphics," says Mr. Krogh. "Students will be taught how to write their own visualization programs."

Spring offerings

The spring semester includes courses in technical communications and computer ethics. The ethics course, to be taught by Bruce Suttle of Parkland's philosophy department, is inspired by a similar course at Stanford University. It will be geared "toward understanding the variety of ethical questions in working with computers," Mrs. Christensen says.

Computer Graphics II completes the sequence begun in the fall. Mr. Krogh says it "is a survey course which looks at several different areas in computer graphics." Students will be required to do a project or write a paper in one specific area. "My intent is to give a brief sampling of everything and the project/paper will allow them to learn a subject in depth," he adds.

A weekly seminar with guest speakers is scheduled as well. Some of the speakers will be prospective employers. The seminar will also include placement services and the teaching of interview skills, taught by Sunny Christensen.

The culmination of the program is a paid internship in the spring semester, beginning in 1990. Students will work with BI scientists, practicing visualization with data from a variety of fields. The internship requires 20 hours per week and can be extended to a summer session.

After completing the curriculum, students will be awarded an advanced certificate from Parkland College. They may also apply many of those credits towards a four-year degree from UIUC. Mrs. Christensen says the program would work well as part of a science or engineering major.

Employment opportunities

If the current lack of visualization specialists continues, graduates of the program should be in high demand for jobs. Mrs. Christensen says possible employers include universities and corporations. The fact that visualization can be useful in just about every scientific field makes graduates very attractive to the research community, she adds. According to Mr. Lathrop, NCSA will certainly need more people trained in visualization, as it brings on more industrial partners. He says that the partners would be interested in the graduates of the program.

Nationally, Silicon Graphics, Inc. has agreed to aid in matching graduates and companies. "The Fortune 500 companies are really adopting this simulation ability, which saves them a lot of money," says Mrs. Christensen. Visualization allows these companies to test a product before actually constructing it. For example, the Boeing Company, in designing its 737-300, used a supercomputer to visualize the airflow over the airplane's surface. The Ford Motor Company designed its highly successful Taurus automobile using similar methods. Eliminating the need for building multiple prototypes, visualization techniques saved Ford several million dollars.

Another employment possibility is in the entertainment industry since computer animation is used in television shows and commercials.

Because of the potential benefits to the corporate community, Mrs. Christensen says she would like to see them get more involved in funding the program. "The internship is now paid from Department of Education funds, but in the long run we want industry support," she says.

At this writing, 75 inquiries and 55 requests for applications had been received at Parkland; ultimately, 20 students will be accepted. Mrs. Christensen says that it has been easy to recruit students, and for now they want to keep the program recruitment local. Even when exposure does increase, Mrs. Christensen says that the program would probably accommodate no more than the presently planned number of students. "Due to available resources, we want to keep it to that size," she says.

For further information, contact:

Mrs. Sunny T. Christensen
Program Director
Advanced Certification Program for Visualization Computer Graphics Specialists
Parkland College
2400 West Bradley Ave.
Champaign, IL 61821-1899
(217) 398-2596 ▲

Mark your calendars for User Group Meeting

by Janice Knapp-Cordes, Assistant Training Coordinator

Reserve October 23 and 24 for the Second Annual NCSA User Group Meeting. This year the meeting will be held at the newly opened Beckman Institute.

A new feature will be two days of tutorials that follow the meeting. A hands-on tutorial on Software Development Tools will be offered, as well as classes in advanced UNICOS and autotasking.

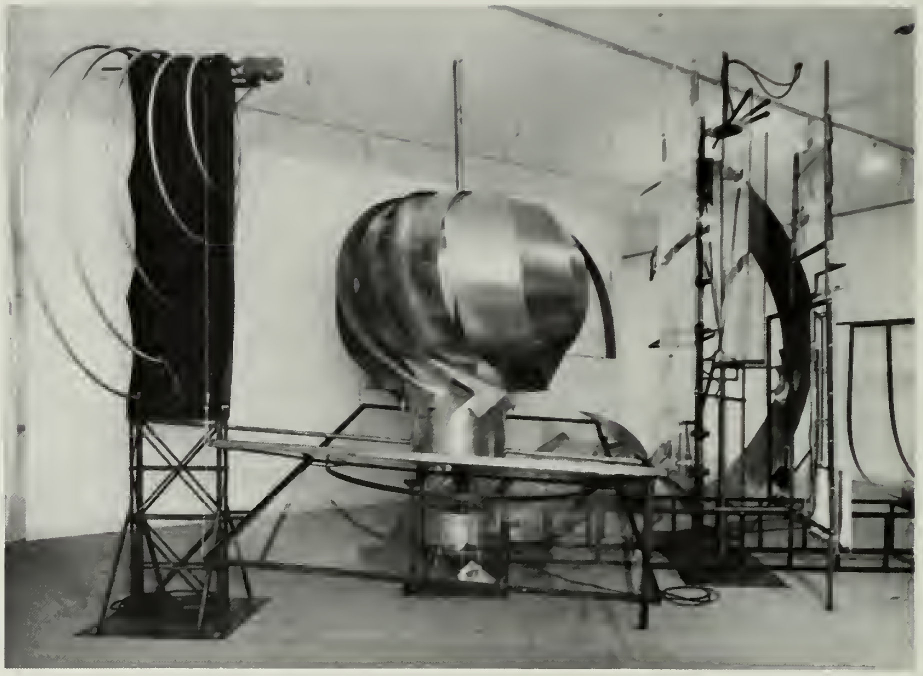
The next issue of ***access*** will contain an article on the meeting together with inserts that include a meeting agenda and a registration form.

Art meets technology

by Fran Bond, Technical Editor

Alice Aycock, one of the most successful sculptors of her generation, spoke recently at the Beckman Institute auditorium. NCSA, together with a number of other campus units, sponsored the illustrated lecture entitled "Alice Aycock: A Sculptor Speaking on Her Work."

Ms. Aycock's works combine historical imagery from a variety of sources—principally science, technology, and art. She introduced her lecture by relating a personal dream experience in which different art historical periods influenced the visions that pervaded her consciousness. The artist called this a "neurological" approach while explaining the format of her talk: a "stream of consciousness" in slides illustrating how she carries out her artwork.



"Hoodo (Laura), Vertical and Horizontal Cross–Sections of the Ether Wind" (Courtesy of Alice Aycock).

Origins of Aycock's imagery

In a mellifluous voice, the artist described the sources of her imagery and influences of her motifs as pertinent slides were projected on the screen behind her. Drawing from vernacular as well as traditional sources, she outlined the effects on her work of countless images including Medieval palmistry notations, WW II war game diagrams, traditional notations from the field of physics, markings for children's games, classical Greek architecture, motifs in Italian Medieval manuscripts, blueprints of naval architecture, amusement park structures, and scholarly textbooks.

Ms. Aycock cautioned that mixing science, mythology, and alchemy—or "magic" as she preferred to call it—can be likened to committing the "Original Sin" which she defined as the human desire to acquire knowledge. One outgrowth of such action, she stated, is making tools, such as arrowheads, to control the environment. She explained that "the desire to know is so strong that we must go on" in spite of the fact that doing so can be "hypnotic," "destructive," and "a danger." Her goal is to combine many sources to express a statement about the influence of technology on mankind.

Evolution of Aycock's works

Ms. Aycock is probably best known for her early, strongly three-dimensional constructions—chiefly in natural wood—suggestive of ancient walled cities or rotating stage sets. The labyrinth is the predominant motif in her works as she explained. Today her sculpture has taken on a more lyrical, almost diagrammatic expression with fewer hard-edge effects. Still working occasionally in wood, she has explored other materials, such as steel and concrete—usually applying paint to the surface of the object.

"Hoodo (Laura), Vertical and Horizontal Cross-Sections of the Ether Wind" (1981) is exemplary of her current style and much of her work. Constructed of a variety of materials, the predominant shape of the piece resembles that of a light bulb standing on its base—the early type with a pronounced bulbous configuration. Ms. Aycock explained that the piece was inspired by an eighteenth century text which was written when electricity and magnetism were being discovered. At that time, she said, some people thought electricity had the property to restore life after death. "Controlled disorder" is how the artist characterizes this work.

Her other works include outdoor as well as indoor pieces—several large-scaled installations utilize a variety of materials. One such piece, "Collected Ghost Stories from the Workhouse" (1980), a permanent outdoor installation at the University of South Florida in Tampa, combines her early labyrinthine motifs of concentric circles with the linear quality of her latest work. In this, as in any one work of Ms. Aycock's, the viewer is immediately made aware of a multiplicity of references.

Multidisciplinary endeavors

With its interdisciplinary approach to scholarship, the BI was an appropriate setting for the lecture of an artist working from multidisciplinary sources. Dr. Jonathan Fineberg, art history professor in the School of Art and Design, initiated the arrangements for Ms. Aycock's appearance on campus.

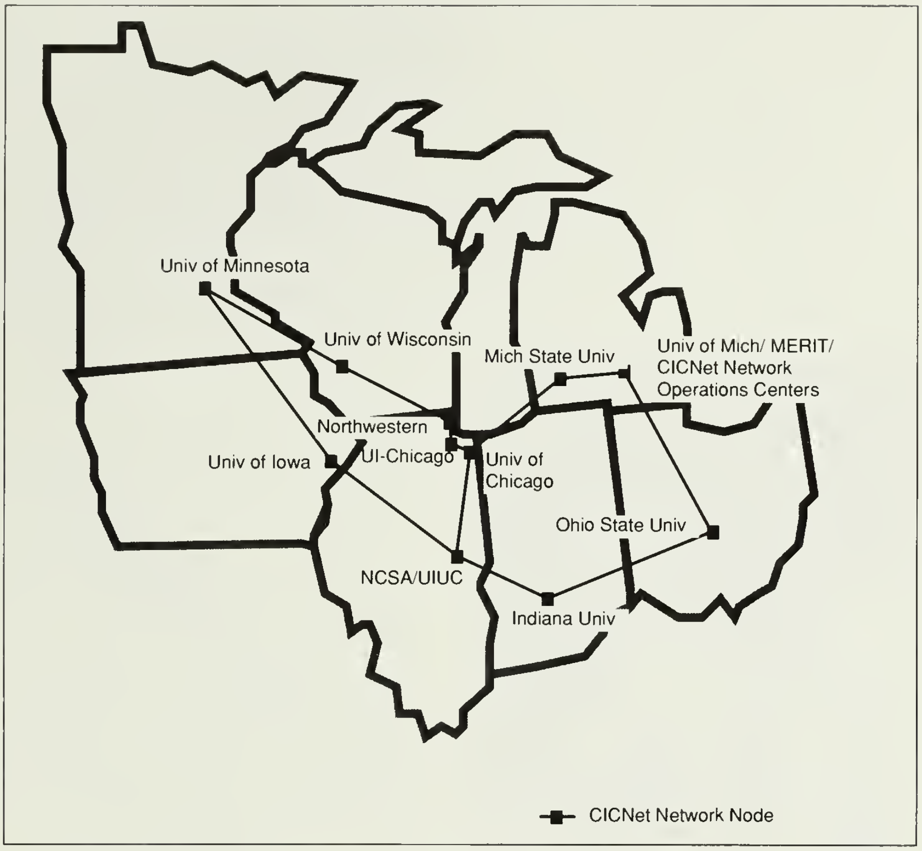
Art *continued on page 26*

CICNet: a new NSFNET mid-level network

by Joel Maloff, Executive Director, CICNet and Charlie Catlett, Manager, NCSA Networking

This year, March has not only been the harbinger of spring, but also witness to the emergence of a new regional research network—CICNet. CICNet is an outgrowth of the Committee for Institutional Cooperation (CIC), a consortium of Big Ten universities plus the University of Chicago.

CICNet links most of these institutions together via leased T-1, 1.544 Mbps facilities (see the CICNet figure, right). As a regional network, CICNet provides mid-level access for researchers between campus and state networks and the national NSFNET backbone. The NSFNET backbone connects CICNet, and the institutions it serves, to other similar regional networks, including MIDnet, Sesquinet, NYSERNet, NCSAnet, and others. CICNet connects to the NSFNET backbone at NCSA and at the University of Michigan.



CICNet links the members of the CIC consortium.

Multicampus network

Most of the campuses connected to CICNet have been part of other mid-level networks in the past. CICNet, however, provides these campuses with higher network bandwidth in most cases and multiple network links in all cases. The multiple links not only double the effective network capacity to each campus but also provide a significant level of redundancy. Should equipment or circuits fail, access to each campus is maintained with the second link. Several campuses—the University of Chicago, Northwestern University, and Indiana University—were previously connected to the NSFNET backbone network through NCSAnet. While NCSAnet provided high bandwidth T-1 facilities, the migration to CICNet brings these campuses redundancy as well, thus improving overall performance and reliability.

The transition from existing network connections—for example, NCSAnet—was done transparently in late February and early March. Thus, users who have previously used NSFNET or accessed NCSA using such applications as telnet or FTP will notice improvements in performance in many cases.

Having been in the implementation stages since the fall of last year under the direction of Executive Director Barbara Wolfe, CICNet became fully operational during the first week of March 1989. Coincidentally, Ms. Wolfe has now turned over the management of CICNet to the new executive director, Joel Maloff. Mr. Maloff brings a new perspective to CICNet, having spent the previous fifteen years in various aspects of the telephone industry. His experience includes ten years within the Bell system and the past three years with the fiber optic carrier consortium, NTN (National Telecommunications Network). His experience in the Internet environment includes extensive work with SURAnet and NYSERNet, as well as input into research network legislation planned by Senator Albert Gore of Tennessee.

Future plans

Plans for CICNet include the development of a business plan with solid objectives and strategies. Among these are plans to

- enhance the understanding and services to users,
- clarify methods of operation, and
- expand the influence of CICNet institutions in the exciting evolution of NCSA's national research network resources.

For information regarding CICNet, users are encouraged to contact their NCSA Affiliate Coordinator or to send electronic mail to

network@ncsa.uiuc.edu (Internet) or
network@ncsavms (BITNET). ▲

Industrial Program happenings

by Larry White, Assistant Director, Industrial Program

Eli Lilly and Company and Motorola Inc. have recently placed two new full-time people at NCSA: Michael Heathman and Margaret Nadworny.

Michael Heathman, Eli Lilly and Company

Michael Heathman.

Margaret Nadworny.

Mike received his bachelor's and master's degrees from the University of Wisconsin—Madison before joining Lilly in 1987. His master's thesis in Physical Chemistry was based on studies of the vibrational energy transfer in gaseous Deuterium Fluoride. He got started with computational models of vibrational and rotational energy transfer first by porting computational codes and later by developing new codes for these simulations.

At Lilly, Mike has worked in the Vibrational Spectroscopy Laboratory performing analytical infrared and raman spectroscopy, before coming to NCSA. In the Spectroscopy Lab, he began using MOPAC software to calculate fundamental vibrational frequencies and displayed these using Bob Hermann's Flick program.

On March 31, 1989, Mike was assigned as Lilly's Scientific Systems Analyst onsite at NCSA. He is the primary liaison between Lilly researchers and NCSA; as he states it, his job is to "be sure the people at Lilly can do the research they want to at NCSA." Over time he hopes to learn enough of NCSA's operation to be able to extract and transfer appropriate parts of NCSA's technology, particularly in visualization, back into the Lilly research laboratories.

Mike reports to Riaz Abdulla, who continues as manager of Eli Lilly Supercomputing Applications, but now works primarily in Indianapolis.

If you are an industrial user at Lilly and need to contact Mike, his phone number is (217) 244-7687. Electronic mail will get to him on the Cray systems at u32063.

Margaret Nadworny, Motorola Inc.

Margaret received her bachelor's in Math from Florida State University, and her master's in Applied Mathematics from the University of Maryland. She joined Motorola in 1984 and has supported process and device simulation in the Bipolar Technology Center (BTC) of the Semiconductor Products Sector of Motorola.

Since 1985 she has been involved with high-performance computing systems—first with an FPS 164, later with a Multiflow, and now with NCSA's Cray systems. Besides using and supporting applications on these systems, she has programmed applications for online statistical process control and defined factory simulation applications for BTC's fabline.

Starting in February, Margaret has been Motorola's Engineering Applications Liaison on site at NCSA. With high goals for Motorola involvement at NCSA for the coming year, Margaret is specifically concentrating on the variety of applications needed for Motorola users, and on reaching out to Motorola engineers who could make good use of NCSA's facilities, but who are not yet participating in the center.

If you are an industrial user at Motorola and need to contact Margaret about engineering applications or using the Cray systems, her phone number is (217) 244-0265. Questions about training, networking, and systems should be directed to Randall Luneack, in the same office, at (217) 244-0264. Electronic mail on the Cray computers will reach Margaret at u33013. Electronic mail for her within Motorola should go to post account ASTF51 on macceng. Randall's Cray computer address is u33006, and his Motorola address is post account ASTF46 on macceng. ▲

UWM students use NCSA's supercomputer

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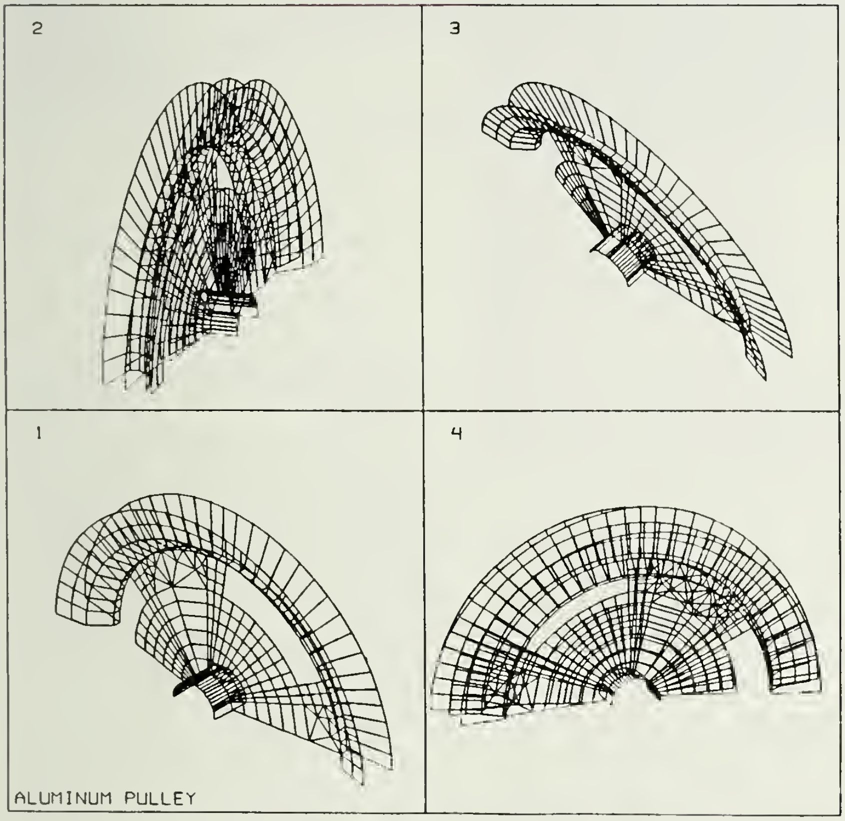
edited by John S. Sfondilias, Affiliates Program Coordinator

At the University of Wisconsin—Milwaukee (UWM), two classes of undergraduate and graduate students are using a National Science Foundation-donated CRAY X-MP/48 supercomputer at UIUC. Professor Mohamed Ahmad's students in engineering are using the ANSYS finite element analysis program. Prior to running on the Cray, they learned the package on microcomputers.

ANSYS finite element model of a pulley deforming under load (Courtesy of David Stack, University of Wisconsin—Milwaukee).



Professor Ahmad continually looks for additional computing power for his students so that they can tackle larger problems. Unfortunately, no finite element packages are available for either of CSD's (Computing Services Division, University of Wisconsin) academic computers. The availability of ANSYS on the CRAY X-MP at NCSA provided the opportunity Professor Ahmad was looking for.

Since the semester was already underway when the situation arose, it was imperative to get students from both classes started on the Cray as soon as possible. After many hurried phone calls and electronic mail messages between Professor Ahmad, CSD, and NCSA, it was decided that the quickest option was to allocate supercomputer time to Professor Ahmad's classes from the UWM Block Grant.

NCSA's Affiliate Block Grant is a pool of supercomputer time which faculty and researchers can draw upon for start-up, training, and educational purposes. Professor Ahmad is the first UWM professor to draw upon this resource for instructional use.

"The assignment the students have in hand right now takes about 32 seconds of CPU (on the Cray)," says Professor Ahmad. "You have to keep in mind that students usually do not solve the problem right on the first trial. This problem takes about 3 hours on a VAX station GPX. I am right now working on other problems which we could not solve before with our limited capabilities. One other note—in both courses I am teaching, students are required to submit a final project. Students have the freedom of choosing their projects. I am sure that during the final project period we will consume a good chunk of CPU time."

ANSYS generates graphic output which can either be viewed on a Tektronix graphics terminal or plotted on a Hewlett-Packard pen plotter. Since there are few of these devices available, Statistical Consultant Frank Stetzer took the UNIX hpglplot filter, which converts plotter commands to laser printer commands, and modified it to accept the format of the ANSYS graphs. Now the ANSYS graphics can be downloaded from the Cray to UWM's UNIX system, and printed on its laser printers. ▲

David Thompson, SDG programmer/project leader with his winning program.

NCSA X Image—a winning window system

by Ann Stowell, Product Coordinator, Software Development Group

Two undergraduate employees for NCSA's Software Development Group (SDG) recently had an opportunity to demonstrate their talents and contributions to science and engineering at the University of Illinois' Engineering Open House (EOH).

Engineering Open House attracts thousands of students, educators, and interested people from all over Illinois annually. For over 35 years, its mission has been to educate the public about engineering in general and about the exciting engineering projects that take place on the UIUC campus. In accordance with this year's theme, "Reviving the Dream," EOH participants demonstrated how UIUC engineering departments and students are recapturing the innovative, entrepreneurial spirit that founded America.

Dave Thompson wins EOH award

Among this year's EOH participants was NCSA employee Dave Thompson—a student in computer science—who earned first place for his prerelease version of NCSA X Image, a versatile and comprehensive color imaging and data analysis software tool designed to run under the X Window System. Project leader for the development of NCSA X Image, Thompson entered NCSA X Image in the category, "Original Research by Undergraduates," and was awarded the highest of five awards in that category.

Thompson has been a programmer for the Software Development Group since November 1985. Along with programmer Eng-Whatt Toh, Thompson is leading SDG research in X Window software. He keeps SDG up-to-date regarding the latest developments by participating in national X Window conferences such as Xhibition '88 and the 3rd Annual X Technical Conference.

SDG programmer Dave Whittington, a student in computer science, developed and demonstrated a jet engine simulator as a participant in EOH. Whittington's project simulated temperature and pressure for various jet engines subjected to different conditions. Whittington has worked for SDG since September 1988 and is currently working on NCSA X Image with Thompson.

NCSA X Image for X Window Systems

Thompson's NCSA X Image software combines the functionality of recently released Macintosh tools NCSA DataScope, NCSA Image, and NCSA PalEdit into one application that can run on any system that supports the X Window System, such as a Sun, DEC, or IBM RT workstation.

NCSA X Image allows users to view and manipulate data values, including datasets calculated on the CRAY X-MP system and digitized pictures. NCSA X Image reads datasets from Hierarchical Data Format (HDF), raw raster, and raw palette files and displays them as actual data values in spreadsheet form, full color cartesian and polar images, and black-and-white contour, shaded data, intensity, and 3D plots. In addition, the application has features that permit advanced data analysis and experimentation. For example, NCSA X Image generates histograms of the frequency distribution of data; allows users to create color palettes (cluts) by using a mathematical expression or manual "mixing" to define individual colors; and lets users customize and manipulate color palettes by inverting, compressing, expanding, or rotating color entries within the palette.

NCSA X Image currently runs using the public domain MIT X server, which users say is "a little slow." Consequently, Thompson and other X Window developers are eagerly awaiting the release of Sun's X/NeWS server and Macintosh's color X server—developments which will speed up NCSA X Image software considerably. Whatever the progress of national vendors, Thompson plans to complete the first official beta test version of NCSA X Image by late spring.

Other NCSA work with X Windows

SDG exploration into the possible scientific applications of the X Window System does not end with NCSA X Image. NCSA X DataSlice, a visualization tool that allows scientists to analyze 3D matrices by viewing their component 2D planes, is currently under development by programmer Eng-Whatt Toh. Like NCSA X Image, X DataSlice supports color raster and numeric spreadsheet displays. Using NCSA X DataSlice, users can select and view multiple 2D planes of data, or *data slices*, selected arbitrarily or along the three cartesian coordinate axes—x, y, and z. To enable detailed data analysis and scientific investigation, X DataSlice employs user-defined color palettes to initialize the color hardware and supports fully synchronized mouse selection between numeric values and points in corresponding color raster images. Toh plans to release NCSA X DataSlice for official beta testing later this spring.

Students grow with NCSA

NCSA X Window software is a product of the experimentation, energy, and initiative that student staff members bring to NCSA. Thompson says that NCSA staff have supported and encouraged his interest and research for the X Window System from the first time he installed X on SDG's Sun workstation "just for fun." When Thompson intimated a desire to merge the features of NCSA's

X Image *continued on page 26*

Connection Machine Seminar

At the recent NCSA-sponsored Connection Machine Seminar held at the Beckman Institute, David Waltz of Thinking Machines Corporation presents an overview of artificial intelligence research being done at Thinking Machine's headquarters in Cambridge, MA.

Extending the parallel platform

by Michael Welge, Numerical Consultant

A vital component of NCSA's Parallel Processing Program is to provide the research community with experimental and developmental access to a "garden" of parallel architectures. Through joint agreements with Argonne National Laboratory's Advanced Computing Resource Facility (ACRF) and Syracuse University's Northeast Parallel Architecture Center (NPAC), NCSA extends its parallel platform from multiprocessors and clustered processors to massively parallel and experimental architectures.

Parallel resources now available through NCSA's Parallel Processing Program include:

- Alliant FX/8
- Ardent Titan
- INTEL iPSC Hypercube
- Thinking Machines CM–2
- AMT–DAP
- Encore Multimax
- Sequent Balance

Resources will be allocated through a review process based on formal merit review and will be subject to resource availability at NCSA, ACRF, and NPAC.

To apply for an account on any of the parallel architectures, contact Patricia Wenzel, manager of User Administration, [see **NCSA Contacts**, page 27].

For additional information about NCSA's Parallel Processing Program, contact Michael Welge [see **NCSA Contacts**, page 27].

X Image continued from page 25

Macintosh tools into an X supertool, SDG provided him the opportunity, responsibility, and freedom to design the application. Now, that supertool—NCSA X Image—is likely to be a useful instrument for scientists across the nation and a ground-breaker for new SDG research and productizing of X Window software tools. As with other NCSA software tools, X products will be fully documented released into the public domain.

All of us at NCSA congratulate Thompson for his award and his outstanding work that earned it. ▲

***Art** continued from page 20*

She was the school's major visiting artist during the 1988-89 school year. According to Dr. Fineberg, Ms. Aycock "juxtaposes the language of high technology—which follows rational rules—with irrational statements or intuitive modes of thought. The result is the unleashing of some unexpected insights." Dr. Fineberg then quoted Ludwig Wittgenstein—British philosopher of the early twentieth century—who said that "True philosophy begins when language goes on a holiday." Dr. Fineberg added, "We would like to find a donor who could commission one of Ms. Aycock's works for the university. Illinois' influence in a number of high technology fields and engineering in general would certainly be a natural setting for one of her installations."

The artist was born in Pennsylvania in 1946. She received her bachelor's degree from the Douglas College of Rutgers University in New Jersey and her master's from Hunter College in New York City. While in New York City, she studied sculpture with Robert Morris and Tony Smith. Her works are included in the collections of the Museum of Modern Art and the Whitney Museum in New York City, the Walker Art Gallery in Minneapolis, and other outstanding contemporary collections. Currently, she is a member of the faculty at Yale University.

Other UIUC sponsors of the lecture included: Office of the Chancellor, School of Art and Design, Coordinated Science Laboratory, Department of Landscape Architecture, Beckman Institute, Humanities Council/LAS, Art History Program, Painting Program, Sculpture Program, Unit for Criticism and Interpretive Theory, Center for Advanced Study, and the George A. Miller Committee. ▲

NSB members at NCSA

National Science Board (NSB) representatives Frederick B. Brooks, Jr. of the University of North Carolina (center) and Rita R. Colwell of the University of Maryland (right) listen to Director Larry Smarr (left) describe NCSA's supercomputer facilities during their recent visit in connection with the renewal of the 5-year Cooperative Agreement with NSF. Hosts Dr. Smarr and Deputy Director Jim Bottum guided the visitors through a tour of NCSA's three locations. While at NCSA, Drs. Brooks and Colwell met informally with staff members and interacted with research scientists. They also lunched privately with seven users who represented the following sectors: industrial, remote scientific, post-doctoral research, and graduate/undergraduate students. The NSB is the governing body of NSF and operates much like the board of trustees of an educational institution.

New and updated online information

by Will Ridenour, Online Documentation Editor

You will find a list of UNICOS man pages and help files in the accompanying *Online Documentation for the Cray Systems.* For further information, see the article in the March–April 1989 issue of ***data link***.

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Norman continued from page 5

Norman. "The 3D code will be able to attack a wide variety of problems in astrophysics—not just radio galaxies," says Dr. Norman.

The code they develop is expected to become a standard research tool for astrophysicists. "We call the code development Project ZEUS, after the Greek god of the cosmos. He went around throwing thunderbolts, which are electrical phenomena that create plasma," explains Dr. Norman. "We're working on ZEUS 2D and 3D and all the attendant software for preprocessing and postprocessing."

The ZEUS postprocessor is already in widespread use. Developed by Dr. Norman and Research Programmer Carol Song as ImageTool for the Sun workstation, that code was further developed by the NCSA Software Development Group and modified for the Macintosh. It is now called NCSA Image [see ***access*** March–April 1989]. Judging from the response to the postprocessor portion, the entire ZEUS project is likely to be a great success.

So, "Yes," agrees Dr. Norman in response to a question, "the six-month dissertation delay back in 1979 seems to have been worthwhile." ▲

Training sessions

Upcoming training sessions are as follows:

1989

June 5–8	New User Training
Sept. 25–28	New User Training
Oct. 30–Nov. 3	Academic Affiliates Training
Nov. 13–16	New User Training
Dec. 11–14	New User Training

NOTE: To attend NCSA training, you must register no later than one week in advance. Class size is limited and these dates are subject to change. To register, contact Kendra Reasor at (217) 244-1100. For additional information about NCSA's Training Program, contact Alan Craig, manager of Training [see **NCSA Contacts**, page 27].

data link Preview

Notes and quick tips

Hot topics in the NCSA Consulting Office
by Chip Mayse, Student Consultant

UNICOS software applications update
by Mark Straka, User Consultant and Mike Krogh, Industrial Consultant

qu database query utility available on the NCSA Cray systems
by Connie Falk Milosevich, UNICOS Systems Programmer

Dynamic memory allocation on the NCSA CRAY-2 system
by Ilhan Dilber, Industrial Consultant

FIDAP 4.20 now available on NCSA Cray systems
by Ramesh Jayaraman, User Consultant

NCAR GKS on NCSA Cray systems
by Rick Kufrin, Systems Consultant

ECMFFT package available on NCSA Cray systems
by Beth Richardson, Applications Programmer

ELLPACK installed on NCSA Cray systems
by Ramesh Jayaraman, User Consultant

NAGLIB Mark 12 available on NCSA Cray systems
by Beth Richardson, Applications Programmer

SPSSX available on the NCSA CRAY X-MP/48 system
by Beth Richardson, Applications Programmer

PC file transfers
by Heeren Pathak, Software Development Programmer

If you want to receive a copy of the current ***data link***, contact the NCSA receptionist at (217) 244-0072.

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the NCSA newsletter

July–August 1989 vol. 3 no. 4

Visualization

NCAR–NCSA collaborate on greenhouse effect study

by Fran Bond, Technical Editor

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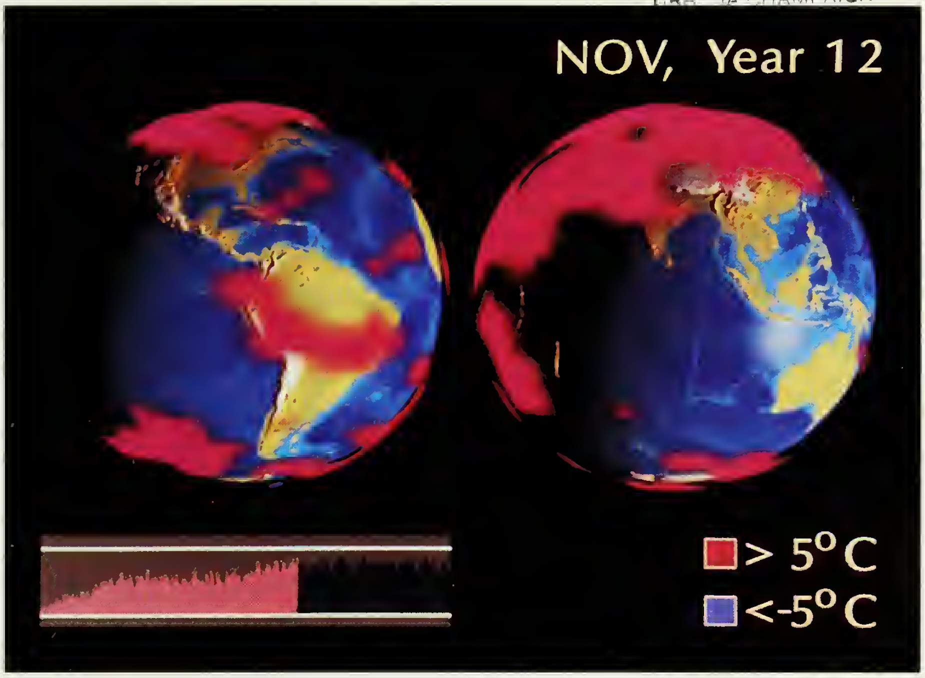

Simulation of global warming due to doubled levels of CO_2. Year 1 is the point at which the doubling occurs, and this view shows Year 12. The graph in the lower left corner shows the resulting warming trend over the 20-year simulation. The red areas on the globe indicate a temperature increase of 5°C or more (Courtesy NCSA Scientific Visualization).

> We stand now in the place and limit
> of time
> Where hardest knowledge is turning
> into dream,
> . . . .
> One or another nightmare may come
> true,
> And what to do then? What in the
> world to do?
>
> *Howard Nemerov,*
> *U.S. poet laureate, "Magnitudes"*

These haunting words from Howard Nemerov's poem echo worldwide concern about the future of the Earth. Scientists and laypeople alike worry about the health of the Earth's environment as each dire discovery or severe weather pattern becomes a media event. Scorching droughts and other environmental disasters of the summer of 1988 mobilized Dick Thompson, Washington correspondent of TIME magazine, to organize The Environment Conference held at Boulder, CO the following November. Political leaders and scientists from five countries, including Russia, convened at the National Center for Atmospheric Research (NCAR) to follow an agenda set by the center's staff. As a result, the New Year's issue of TIME focused on "Endangered Earth as Planet of the Year" instead of the usual "Man/Woman of the Year" [see *TIME*, January 2, 1989].

The greenhouse effect is one major "nightmare" mentioned in Mr. Nemerov's poem. According to some scientists, this phenomenon is beginning now—not in the twenty-first century, as others forewarn. In a report to the U.S. Senate Energy and Natural Resources Committee last summer, climate scientists reported that global warming may be occurring, but the evidence is still unclear.

Greenhouse gases

For some years, mathematical models have foretold that a buildup of carbon dioxide (CO_2), found in fossil fuels such as coal, and other gases, activated by mankind's activities such

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Abbreviations

CRI	Cray Research Inc.
IRC	Interdisciplinary Research Center of NCSA
NCSA	National Center for Supercomputing Applications
NSF	National Science Foundation
UIC	University of Illinois at Chicago
UIUC	University of Illinois at Urbana-Champaign

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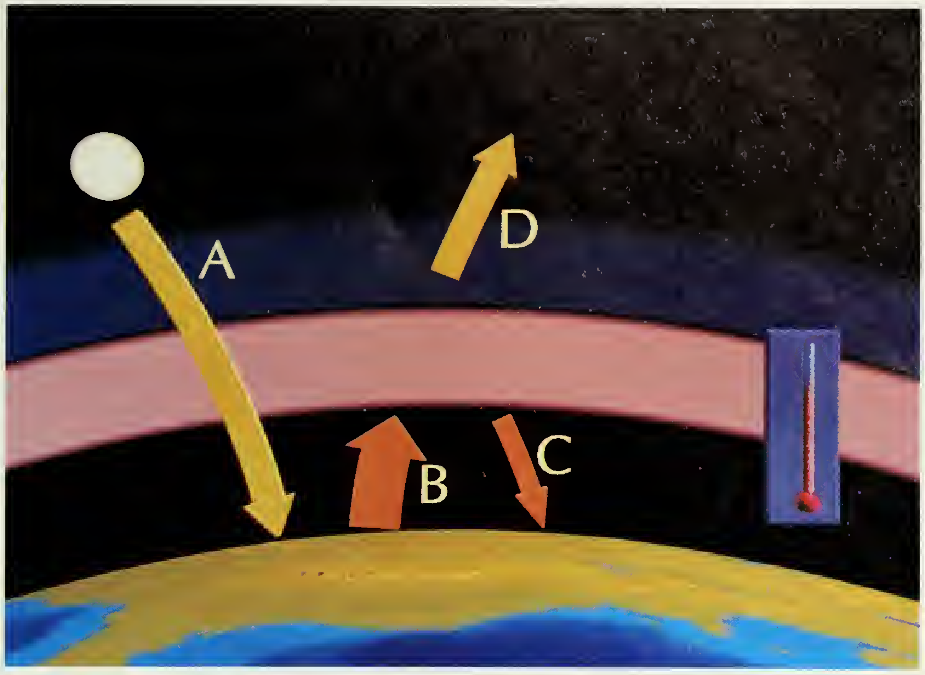
The greenhouse effect. Incoming radiation at A is absorbed by the Earth and reemitted as terrestrial radiation at B. A portion of this is absorbed by the greenhouse gases (shown in red) and radiated back to the Earth at C. Although all incoming radiation is balanced by the outgoing radiation at D, it is the cycle indicated by the B and C arrows which causes warming in the lower atmosphere and cooling in the upper atmosphere (Courtesy NCSA Scientific Visualization).



Greenhouse *continued from page 1*

as the use of refrigeration coolants, will cause the Earth's surface to warm. By absorbing more of the radiation emitted by the Earth's atmosphere, these gases—commonly called "greenhouse gases"—could force a rise in the Earth's temperature.

The Earth's heat balance is maintained through complex interactions with the atmosphere. Incoming solar radiation which is absorbed at the surface is reemitted as infrared radiation. This, in turn, is partially absorbed and reflected back to the earth by greenhouse gases in the atmosphere. A cycle is created in which the Earth and the atmosphere warm each other. Although the final amount of radiation released into space must always equal the incoming solar radiation, increased greenhouse gases intensify this cycle and thus warm the surface of the Earth. Because greenhouse gases absorb more radiation at lower levels, the upper atmosphere is actually cooled. (See the diagram above.)

Carbon dioxide is the major actor in this cycle. Most scientific projections to date assume that roughly one-half of the CO_2 that is released into the atmosphere stays aloft; plants and the oceans absorb the other half. Although it naturally occurs in the atmosphere, CO_2 has increased markedly since the dawn of the Industrial Revolution in the early 1800s. By studying air trapped inside glacial ice, scientists have documented this rise in CO_2.

Because of the Earth's sensitive balance, it is thought that global warming of only a few degrees could have a profound effect worldwide. (For example, during the most recent Ice Age, the Earth's average temperature is thought to have been only 5° C colder than now.)

The Earth and its people form an interactive ecosystem that works much like the proverbial *House That Jack Built* on the scale of a macrocosm. Global warming has the potential for dire consequences worldwide by causing droughts in previously fertile areas, flooding in coastal regions, and conditions that allow certain pests and weeds to flourish at an unprecedented level. These ecological changes could in turn lead to political and social upheavals as the economic bases of various geographical regions shift. Sudden climatic change would be even more devastating.

Scientists cannot agree on the details: how much warming has already happened, what levels of warming are due in the future, or what effect this warming will have on the Earth's climate. Neither do all foresee a uniform ecological Armageddon. But scientists do concur that the atmospheric level of CO_2 has risen, that this level is increasing quickly, and that the Earth's populace is in the midst of a heretofore unknown perilous race with time.

Collective evidence points to inevitable climatic change through global warming, according to the United Nations Environment Programme based in Nairobi, Kenya.

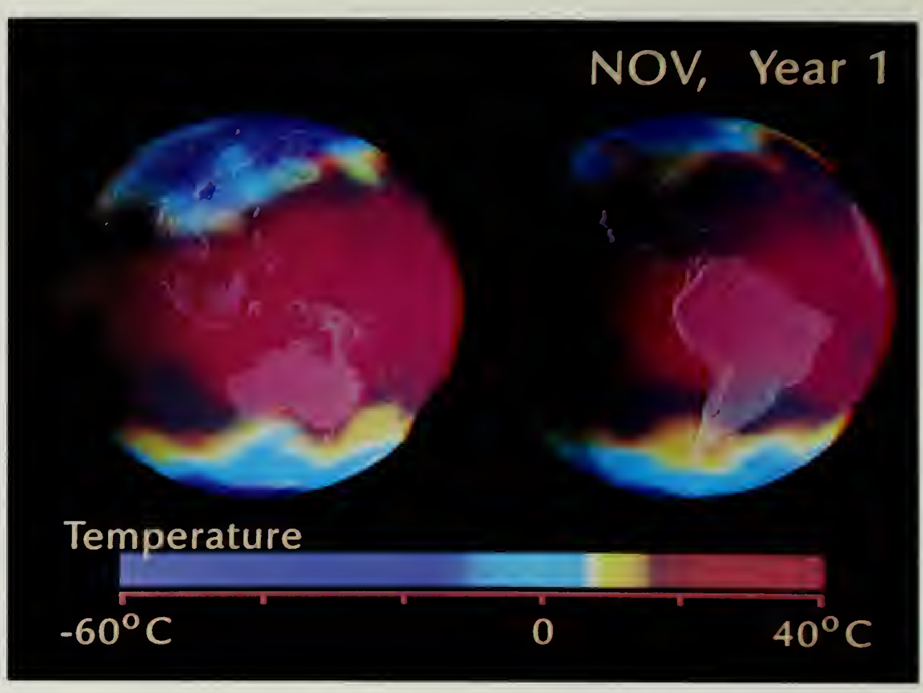
Since the major fear is of sudden, cataclysmic change, scientists today are vigorously seeking the answers to questions like "How soon?" and "How warm?"

Modeling global climatic change

Scientists at NCAR's Climate and Global Dynamics (CGD) Division have had a long-term research interest in the greenhouse effect. Through computer models called General Circulation Models (GCMs), NCAR investigated the Earth's possible climatic response to an increase in greenhouse gases.

NCAR modeled and experimented with its data in a two-pronged effort. One experiment (Experiment A) was developed to show what would happen if no global environmental changes were made in the status quo for 20 years. Another (Experiment B) depicted what would happen in 20 years if the current atmospheric level of CO_2 was suddenly doubled. By taking the difference between the two experiments, the effects of an increase in CO_2 could be found.

Greenhouse *continued on page 4*



Climate simulation at current CO_2 levels for an arbitrarily numbered Year 1. Temperature is color-coded as indicated. North America, experiencing winter as it is blanketed with a layer of cold blue, is in the upper right-hand corner (Courtesy NCSA Scientific Visualization).

Greenhouse *continued from page 3*

NCAR's goal was to determine the steady-state, or long-term, response to the doubling of CO_2.

Numerical models of atmospheric circulation are complex because they contain many interactions that occur in reality. For example, an oceanic model coupled to an atmospheric model can predict currents, temperature, and salinity in oceans around the globe. General circulation models of quantities the atmosphere and oceans use are computed using the basic laws of physics: Newton's second law of motion (force = mass x acceleration), the equation of continuity (conservation of matter), and the first law of thermodynamics (conservation of energy). Since these models are computationally complex, very large computers are needed to derive realistic solutions.

NCAR's atmospheric model was fully three-dimensional and went to nine levels vertically. The horizontal grid was 48 longitudinal points x 40 latitudinal points. Realistic geography, solar and terrestrial radiation, clouds, precipitation and evaporation, soil moisture, snow cover, and sea ice were represented. The oceanic model was a simple, mixed layer.

NCAR's computer simulations were compared with observational evidence. Visualizations were needed to meaningfully convey NCAR's data on climatic changes, and that is where NCSA came onto the project.

NCAR contacts NCSA

Warren M. Washington, director of NCAR's Climate and Global Dynamics Division (CGD), contacted NCSA's Scientific Visualization and Media Services Group in the fall of 1988 to collaborate in the production of a videotape on the simulation of the greenhouse effect. Increasing demands from the government, public, and media for NCAR to present its computer experiments in an understandable format motivated this project.

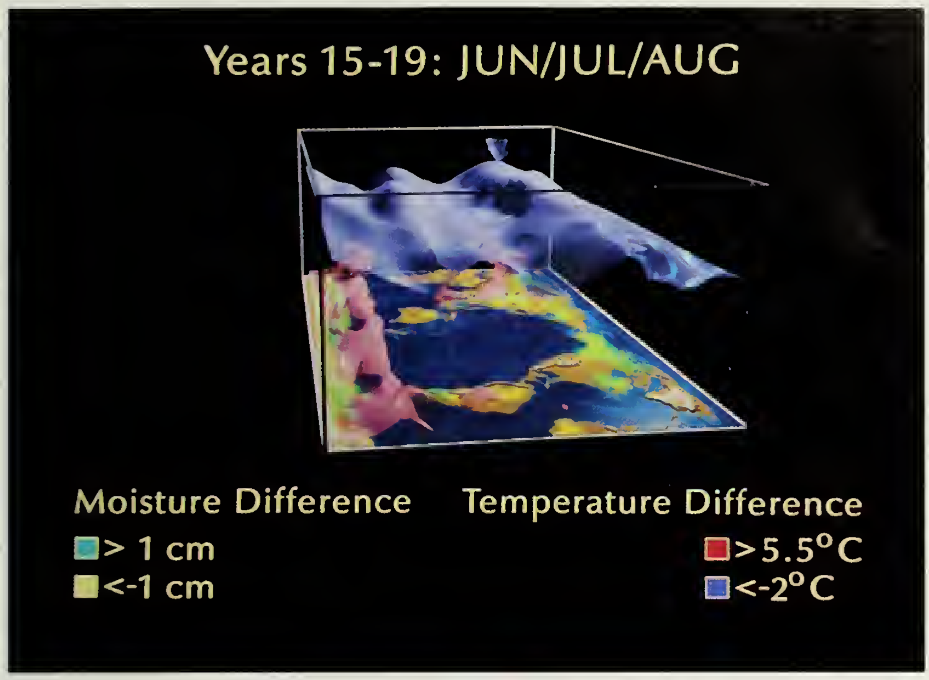
NCAR had been making computer movies for more than 20 years. According to Dr. Washington, NCAR's visualization equipment had not "kept up with video technology; however, in the future it hopes to become state-of-the-art in video animation production." Therefore, NCSA was asked to visualize NCAR's data. NCAR's job was to specify the concepts to be visually conveyed, while NCSA's task was to produce a visual definition of NCAR's findings.

Work on this project began in January 1989. It was initiated by a telephone conversation between Jeffery Yost, scientific animator at NCSA, and Thomas Bettge, a part of the research effort from NCAR's Climate Sensitivity and CO_2 Research Group. Since simulations had already been run at NCAR, Mr. Yost received some sample data on magnetic tape shortly after the phone call. It was accompanied with an extensive written description of what NCAR wanted to show with the project. Work then began in earnest to produce a series of test visualizations that were mailed to NCAR for review.

In March, Dr. Washington, Mr. Bettge, and Don Middleton, computer graphics specialist at NCAR, flew to Champaign to discuss the project in more detail. During this two-day meeting, modifications were made to the visualization techniques, new techniques were proposed and discussed, and a schedule was developed for completion of the project.

After the CGD group returned to Boulder, Mr. Yost continued to produce and mail test videotapes to NCAR. Mr. Bettge communicated with NCSA via electronic mail after the tapes were reviewed in Boulder. In addition, Mr. Bettge was able to develop color palettes using NCSA Image software, an application developed by NCSA's Software Development Group, which Mr. Yost then retrieved over the network. "It was a powerful tool that allowed precise communication," says Mr. Yost. "It's much better than trying to describe colors over the phone!"

According to Mr. Yost, the testing and development phase of the project was the longest. In late April, Mr. Bettge returned to Champaign with final data and some software. He and Mr. Yost divided their time between testing and discussing the videotape's script. By the time Mr. Bettge returned to NCAR, a complete story



Summer temperature difference averaged over five years, displayed as three-dimensional contours above a flat Earth. The regions below the red surface are warmed by 5.5° C or more, while the regions above the blue surface are cooled by 2° C or more. Superimposed over the Earth are areas of moisture increase (shown in green) or decrease (in yellow) due to doubled CO_2 levels (Courtesy NCSA Scientific Visualization).

board, or scene-by-scene written and pictorial description of the visualization, had been developed. This story board was closely followed in the completion of the project.

Publication of the project

In early 1990, the videotape may be featured in an issue of the *International Journal of Supercomputing Applications*. The description of the project would include printed matter as well as a special videotape supplement. At press time the videotape, together with a paper by NCAR, had been submitted for review.

NCAR is operated by the University Corporation for Atmospheric Research and is sponsored by NSF. In addition to Dr. Washington and Mr. Bettge, collaborators from NCAR included Gerald A. Meehl and Lynda VerPlank. A portion of this study was supported by the Carbon Dioxide Research Program of the Office of Health and Environmental Research of the US Department of Energy. The National Magnetic Fusion Energy Center at Livermore, CA provided computational support. ▲

Science

NCSA Computational Chemistry User Group

by Sam Milosevich, Industrial Consultant

The auditorium of the newly opened Beckman Institute for Advanced Science and Technology (BI) was the site of the recent NCSA Computational Chemistry Users Group Meeting on April 20. After an introductory business session, academic users and industrial partners were treated to a lecture on "Large-Scale Electronic Structure Calculations (How Big Is 'Big'?)" by Professor Jan Almlöf of the University of Minnesota and the Minnesota Supercomputing Institute.

NCSA Chemistry Group activities report

Members of the NCSA Computational Chemistry Group made brief presentations.

Drs. Joe Golab, applications scientist in chemistry, and Sam Milosevich, NCSA industrial consultant to Eli Lilly and Company, commented on applications software available now and expected soon on the UNICOS CRAY-2 and CRAY X-MP/48 systems. Dr. Nora Sabelli, research scientist and Education coordinator, summarized the education program which she is organizing to assist NCSA user sites that wish to incorporate curriculum modules into educational courses and training classes. Dr. Harrell Sellers, head of the NCSA Computational Chemistry Group, exhibited his latest desktop visual-ization efforts which pass wave function output from the MOLECULE-SWEDEN computational program for processing and display by a trio of NCSA workstation utilities: NCSA Contours, NCSA DataScope, and NCSA Image.

Large-scale electronic structure calculations

Professor Jan Almlöf focused his lecture on methods for "SCF and beyond SCF." He is well-known for his work with self-consistent field (SCF)

Chemistry Users *continued on page 25*

Clouds with silver (iodide) linings

by Kathleen Robinson, Science Writer

At 10 a.m. most mornings this summer, about a dozen people—scientists and pilots—crowd into a room in a quonset hut at the University of Illinois' Willard Airport.

Against the backdrop of a persistent printer updating the latest weather bulletins, Bob Scott, chief forecaster for the PACE '89 project, begins the day's prediction. His purpose is to find some developing clouds for these pilots to fly *into*. Uneventful weather has kept them on the ground for several days. The meteorologist plays to the mild suspense in the room, pausing melodramatically before he turns over a piece of cardboard that leans against the map on the wall. The other side of the card is fluorescent orange, with "Go" scrawled upon it in large letters. Team members break into laughter, then the discussion turns to instrument readiness and the flight condition of the two planes that will be going up today.

PACE, which stands for Precipitation Augmentation for Crops Experiment, is one of the ongoing research projects carried out by the Illinois State Water Survey (ISWS). The purpose of the PACE project is to determine whether the types of clouds found in the Midwest can be successfully seeded with silver iodide to increase rainfall. The cloud seeding technology, which was first developed in the 1940s, gained new public interest last year as a possible remedy to the drought. However, the effectiveness of cloud seeding remains unproven from a scientific point of view.

Experiments with silver iodide

Silver iodide seems to accelerate the rate at which supercooled water droplets become ice crystals in a cumulus cloud. Heat released in the process may make clouds more buoyant, leading to larger or longer-lasting clouds which have the potential, at least, for more precipitation.

Research with weather modification in Florida seems to have been successful during some years. There also are indications that cloud seeding works in the Israeli climate and in the winter clouds of the American West. Operational projects done in Illinois in the 1970s seemed promising, but they were not carried out with scientific controls.

With funding from the federal government administered through NOAA (National Oceanic and Atmospheric Administration), the ISWS team has devised an experimental protocol that includes the use of placebos (sand flares) as well as flares of silver iodide. The team members do not know whether they have seeded a cloud with silver iodide or the inert sand. In a 1986 field project, they tracked storm activity in 20 clouds. This summer they hope to fly through 100 clouds, weather permitting.

Personnel and equipment

The PACE '89 project is headed by Stan Changnon of the ISWS. Bob Czys, operational coordinator and the aircraft meteorologist, goes up on the flights. Nancy Westcott, director of radar operations, works from a semi-truck trailer that houses the radar and communications equipment. From this base, she and the other scientists on the ground communicate with those in the plane—advising them by radio of promising weather developments. (The project was granted a temporary radio license from the FCC.)

Also on the team are Bob Scott, chief forecaster; Floyd Huff, seeding officer; Eugene Mueller, CHILL chief radar engineer; Dave Brunkow, radar engineer; Jerry Nespor and Don Staggs, HOT radar engineers; Norm Ostrander, chief pilot of the Beechcraft Baron; and Dennis Musil, operational director of the T-28 aircraft loaned by the South Dakota School of Mines and Mine Technology for the month of May. The T-28 is armored for use as a storm-tracking plane and can fly at altitudes and in conditions (such as hailstorms) not suitable for other aircraft.

The CHILL radar is one of the top research radars in the country. The name comes from Chicago/Illinois, because it was originally built by the University of Chicago and the University of Illinois. CHILL was refurbished in the last five years by the National Science Foundation and now is a national facility under NSF, the University of Illinois, and the ISWS. In a bit of contrary humor, the ISWS came up with the name Hydrological Operational Tool (HOT) for their second weather radar.

Nancy Westcott in the portable radome.

Preliminary results

The 1986 field project led to some interesting results. Says Ms. Westcott, "An important finding was that we could tell which radar echo core was associated with the cloud treated by the aircraft. From that, we knew which echoes to track as we computed cloud growth rate. Out West, after a cloud grows to the 20,000-foot level, it may be five or ten minutes before you see a radar echo. Here water particles will form sooner and at lower elevations because midwestern clouds have more moisture.

"Another finding was how rapidly each of the cumulus congestus clouds joined with neighboring clouds, making it impossible to compute rain from an individual echo core. Rainfall increases from cloud seeding must be determined on the basis of a whole cloud system, not just from the treated

Left T/NSF T-28
(Credit: Bob Czys).
Below left Beechcraft Baron
(Credit: Bob Czys).

cloud. Additionally, in 1986 we did not find the rapid cloud growth sometimes expected from cloud seeding. Rather, in this part of the country, cloud seeding may slow the natural deceleration of a cloud. That is, we may prolong the life of a cloud, but not necessarily make it grow taller."

Massive datasets

Even during severe weather when they do not make cloud seeding flights, the team tracks thunderstorms from the ground, collecting data in five-minute intervals for much of the day. Just one moderately stormy day in May, for example, resulted in *four* 3600-foot 6250 BPI computer tapes, packed full with binary data.

The PACE team uses NCSA's CRAY X-MP/48 system to store some selected datasets that have been preliminarily screened for particular interest. Less interesting data is not transferred to the supercomputer. Software to survey data from cloud treatments and to interpolate that data to a three-dimensional Cartesian grid has been recently adapted for the UNICOS environment.

Tracking cloud growth

The 10-cm radar detects clouds when an electromagnetic beam is reflected by water particles in the cloud. The reflection is referred to as an echo. The larger the particles of water or the more particles there are, the stronger the echo. Radar data is collected in 360° sweeps, at 12 different elevations.

In the analysis phase, the radar data is interpolated on horizontal grids of 1 km x 1 km, in 1-km height intervals. Different programs calculate the area of a shower and its rainfall, but the growth of the individual cloud components inside a shower are of primary interest.

Cloud seeding procedures

Once an appropriate cloud has been spotted, the plane is flown through at about 20,000 feet, releasing flares of either silver iodide or sand (selected randomly, their identity code known to none but the project director and the seeding officer). Onboard instruments record physical variables such as the vertical motion of the air and moisture content of the cloud. From this information, the cloud buoyancy can be calculated. "Using this data," says Ms. Westcott, "we predict what the cloud should do—whether it should continue to grow, to accelerate upwards, or to decelerate. We assume that we have dropped silver iodide and that the cloud freezes, then we compute what effect that should have on the cloud. As far as I know, this is the first time anyone has tried to predict from *aircraft* data how the cloud should grow.

"We're trying to look at the cloud just for its first thirty minutes or so. We want to see if we can predict an initial increase in cloud top height, or the diameter of the cloud, or its buoyancy, or the updraft speed. We also collect radar rainfall data—that is, low-elevation angle reflectivity data—so in future years we'll be able to look and see if perhaps we increased the area the cloud covered with rain. However, there are so many processes involved it is difficult at this point to try to measure any rain effects.

"The natural variability is so large in any given cloud system. To truly find an increase in rainfall, you have to design an experiment differently. There is sizable variability over a few miles and between days in summer rainfall making it very difficult to detect hoped-for increases of 10 to 20 percent. In the last 10 years of weather research, one thing we've realized is just how complicated a midwestern rain system is. We now know that not every cloud will act or react in the same way. Some clouds are more apt to

Clouds *continued on page 8*

Clouds continued from page 7

be favorably affected by seeding material."

Other benefits

The ISWS receives dozens of telephone calls each year from farmers and agricultural organizations who wonder whether cloud seeding works. Last year's dry summer prompted more than 200 calls. "We would like to be able to give people a definitive, scientifically based answer to that question," says Ms. Westcott.

Whether or not cloud seeding proves ultimately to be practical—or even desirable in terms of social, economic, and environmental effects—the research alone has been beneficial. According to Ms. Westcott, "Weather modification projects have supported extensive cloud dynamics and cloud physics research. We've learned a lot about clouds and weather along the way. Just the fact that we're looking at clouds has improved forecasting and increased our understanding of how pollution affects clouds." ▲

Call for publications from NCSA's Cray projects

Research on the CRAY X-MP/48 and CRAY-2 systems has produced interesting and valuable findings in a variety of disciplines. NCSA would like to have copies of publications that have resulted from research projects on the Cray systems.

If you contribute your research results to conferences, journals, books, newsletters, or other publications, please send reprints or copies to Patricia Wenzel, manager of User Administration, NCSA, 152 Computing Applications Building, 605 East Springfield Avenue, Champaign, IL 61820. Contact Mrs. Wenzel by telephone or electronic mail for further information [see **NCSA Contacts**, page 28].

Catalysis by design: computational chemistry

by Kathleen Robinson, Science Writer

"A good way to describe this research would be to call it catalysis by design," says Dr. Harrell Sellers, head of the NCSA Computational Chemistry Group. "One of our long-range goals is to design catalysts for particular chemical reactions using computational methods. Catalysis is of intense interest worldwide—a large percentage of the gross national product actually is based on chemical catalysis."

The research being described by Dr. Sellers is currently focused on transition metals, particularly niobium. "Clusters of niobium metal have a very striking chemical reactivity with respect to the dehydrogenation of organic molecules. Niobium will strip the hydrogens off benzene, for example. Chemical reactivity ultimately depends on the structure and the bonding in the metal clusters, so I'm working now on calculations to determine those. Knowing the structure should allow us to explain the chemical reactivity. There is currently no simple model, no descriptive way of even making an intelligent *guess* at the structure of small metal clusters. So we hope to make some headway in that direction, based on molecular orbital arguments."

Reaching for a small periodic table on his desk, Dr. Sellers indicates the cell representing niobium—element number 41. "With 41 electrons, just the atom alone is a relatively big system. By the time we get three or four niobium atoms together we've got quite a number of electrons to account for. And if we include any other small molecules in the calculation such as methane or nitrogen, we really have quite a large system that current ab initio codes can't treat. Our core project in the chemistry group is to develop programs that will allow efficient ab initio or semi–ab initio calculations on these very large systems. We have some other interesting projects in the area of transition metal chemistry. For example, we are modeling the palladium-catalyzed hydrogenation of carbon–carbon double bond systems, in an effort to understand the interactions that give rise to the catalysis. Also, we are interested in the oxidation of methane and nitrogen.

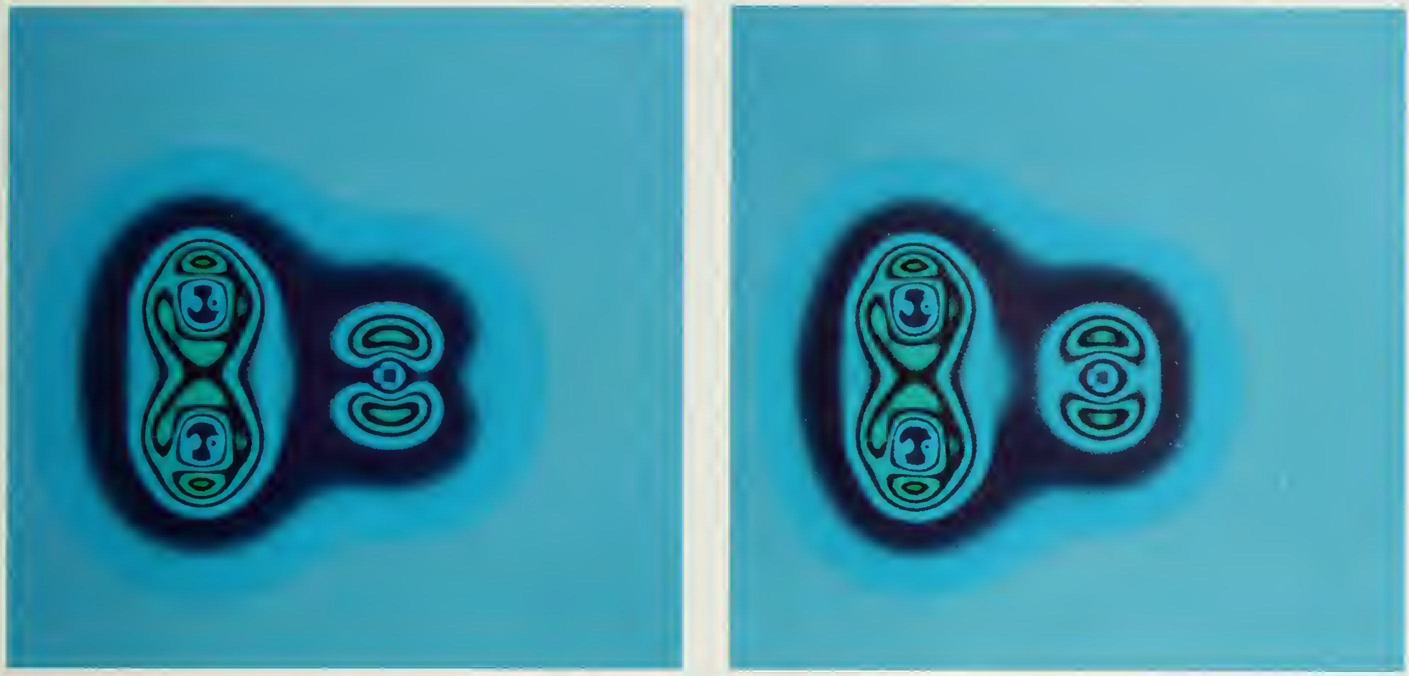
Dr. Harrell Sellers.

"Of course," he adds, "personal research interests drive our efforts to develop such a suite of codes. But when we do, they are available at no charge to the NCSA industrial partners as well as the other NSF centers and the usership in general."

Members of the group

The Computational Chemistry Group at NCSA consists of Dr. Harrell Sellers, head; Dr. Joe Golab, applications scientist in chemistry [see ***access***, March–April 1989]. Dr. Nora Sabelli, senior research scientist whose main responsibilities are education and training at NCSA and quantum chemistry research [see ***access***, May–June 1989], is a contributing member of the group. Dr. Sam Milosevich, consultant for NCSA industrial partner Eli Lilly and Company, also is involved. Other NCSA chemists peripherally involved include Dr. Gail Golab, visiting research chemist, and Ms. Hui Yu, student programmer. Although not a chemist, Dr. Radha Nandkumar, applications programmer, has made many valuable contributions to the group.

Two views of the ionization of the niobium 3 (Nb_3) molecule. The ab initio electron density in the plane of the three nuclei of the neutral (left) and cation (right) is shown (Courtesy Harrell Sellers).



When I ask about the group's range of activities, Dr. Sellers launches into a list: "We're doing the transitional metal chemistry. We're doing method development in the protein modeling area, and method development as relates to the parallelization of large ab initio codes. We're doing quite a bit of quantum chemistry visualization. We maintain the library of chemistry programs here, and we consult with users—*a lot*. We advise them about methods and how to implement those methods."

Quarterly user meetings

With well over 200 accounts at NCSA attributed to chemistry, Dr. Sellers finds that advising chemistry users requires a significant effort. "As more people use our programs, the need for training grows. Many chemists are perfectly happy to run programs as a 'black box' and hope for the best, but others are not—they want to know what the programs are doing."

The Chemistry Users Group meets quarterly and usually has a speaker of national renown at its meetings. (See page 5 of this issue for the news of the most recent meeting.) Alison Howard from Peter Kohlman's group came in 1988 to talk about biomolecular modeling programs. Warren Hehre spoke in December 1988 about his suite of optimized programs [see ***access,*** January– February 1989]. Jan Almlöf from the University of Minnesota spoke in April 1989 about methods for doing very large ab initio calculations. At the user group meetings, NCSA scientists also update users about the status of the library of chemistry codes and current developments at NCSA.

The next Chemistry User Group Meeting will be held in late summer or early fall of 1989. That meeting may be in the form of a two- or three-day workshop. Details will be announced in VAX notesfile CHEMISTRY. (To access that file, simply log on to the VAX front-end machine [ncsaa or ncsab] and enter `NOTES`. The chemistry conference can then be accessed by entering `OPEN CHEMISTRY`.) (See ***data link,*** September-October 1988 for details on using VAX notesfiles.)

Dr. Sellers would like to encourage more use of the chemistry VAX notesfile. Says he, "We post every new program that's up, every new development in the chemistry group there. Some of the industrial chemists use it all the time, but not many of the academic users."

Quantum visualization results

When asked about the quantum visualization work he mentioned earlier, Dr. Sellers turns to the workstation on his desk saying, "Let me *show* you some of the chemistry visualization." He searches quickly through a list of images, then finds what he is looking for. "This two-frame animation sequence shows the ionization of the niobium 3 [Nb_3] molecule. The first image is the neutral molecule, the next is the ionized molecule. It's kind of a cartoon, but it's from the Schrödinger equation. It's not hand-drawn—it's actually from the physics."

The animation on the screen before us consists simply of two static images presented one after the other in rapid succession. "First of all," explains Dr. Sellers, "you see that when the molecule is ionized, electrons leave from the whole molecule—the *whole* molecule shrinks, not just one part of it. Also, you can see that with ionization the electron density actually increases between the dimer molecule and the atom. The purple (representing low electron density) goes away and more blue

Catalysis *continued on page 10*

Catalysis *continued from page 9*

(representing high electron density) increases there." He points at the screen.

"So what you see is actually a building up of bonding electron density upon ionization, which is, in a way, counter-intuitive. It means the electron that leaves is leaving from an antibonding orbital." He sits back in his chair, satisfied. "There's just a whole lot of chemistry in that little animation sequence. It shows the chemistry very well. You wouldn't necessarily see all that by looking at numbers in the output. That's what visualization is all about."

Dr. Sellers turns again to the screen to call up another animation. "This is also the niobium 3 molecule, but this little animation sequence shows the electronic excitation from the ground electronic state to the lowest lying excited state. The molecule is absorbing energy and going into a higher quantum state, and we're going to see the changes in the electron density when that happens."

The colored blob on the screen changes almost imperceptibly, but that seems to make sense to a chemist. "Now, as you can see, there's a very *minor* change in the electron density. This atom is essentially just pumping back and forth. You can see a little bit of degradation in the bonding electron density as the molecule goes into an excited electronic state, but not *much*. So actually what this tells me is that the chemistry of these two states ought to be very much the same. There's not much difference in the electron density of these two electronic states of this molecule.

"That is *important*," he responds to my question, "because, ultimately, considerations like this will govern how we model these metal systems. If it doesn't matter whether it is in the lowest lying state or the ground electronic state, then we could perhaps make a method that behaves better mathematically by averaging over those states, without affecting the accuracy of the description."

The animation sequences Dr. Sellers is showing result from an interface that he wrote between one of the ab initio codes and a contouring program. That contouring program was in turn interfaced with the NCSA Image applications program developed by NCSA's Software Development Group [see ***access***, March-April 1989]. Dr. Sellers presented the images at the Midwest Theory Conference in the early spring of this year.

Juggling roles

With the list of computational chemistry tasks in mind, I ask Dr. Sellers how he manages to juggle his different roles.

"It's hard," he admits. "I try to prioritize my work, and some things fall off the end of the list. I sometimes wake up in the middle of the night and log on to the machine from home to see if I need to turn the jobs around. It bothers me to think that those Cray machines might be sitting there with nothing to do."

Idle machines are not a likely prospect, it seems, with computational chemistry on the rise. ▲

Scientific visitors at tea

A recent tea for long-term visiting scientists at the IRC. Mike Norman (left), NCSA research scientist, converses with Giovanni Bachelet (center), physicist, and Walid Abu-Sufah (ear and shoulder at right), computer scientist.

Scientific visitors

Walid Abu-Sufah
May 8–July 8 from Virginia Polytechnic Institute
Area of research: computer science.

Giovanni Bachelet
April 13–July 15 from University of Trento
Area of research: physics.

Ken Bishop
June 1–5 from University of Kansas
Area of research: chemical and petroleum engineering.

Daniel Johnson
June 14–16 from University of Wisconsin—Madison
Area of research: atmospheric sciences.

Parallel and vector processing conference

Conferees register for NCSA's Second Conference on Parallel and Vector Processing held at Jumer's Conference Center, Urbana, IL, May 8–10 (top). David Kuck, director of the Center for Supercomputing Research and Development (CSRD) and professor in the Departments of Computer Science and Electrical and Computer Engineering (UIUC), gave the keynote address, "The Performance of Parallel Computers" (below). Dr. Kuck compared traditional sequential machines of the "Von Neumann era" with contemporary parallel and vector architectures of the "Parallel era." He says that the drive for speed and efficiency can lead to "big machines doing teraflops" together with "little parallel machines on everyone's desk by the mid–1990s." ▲

Conferees respond

"As usual, NCSA delivered. Everyone was friendly and helpful. The planning for this was quite evident. ...Consider your job well done! In general I don't think I wasted my time. I learned quite a few new things."

"I enjoyed the opportunity to meet and speak with others with interest in this field. The fact that we ate lunch and dinner together made it easy to have informal discussions for extended periods of time."

"Enjoyable, relaxed, informative—I'll be back next year if possible."

"The speakers were excellent."

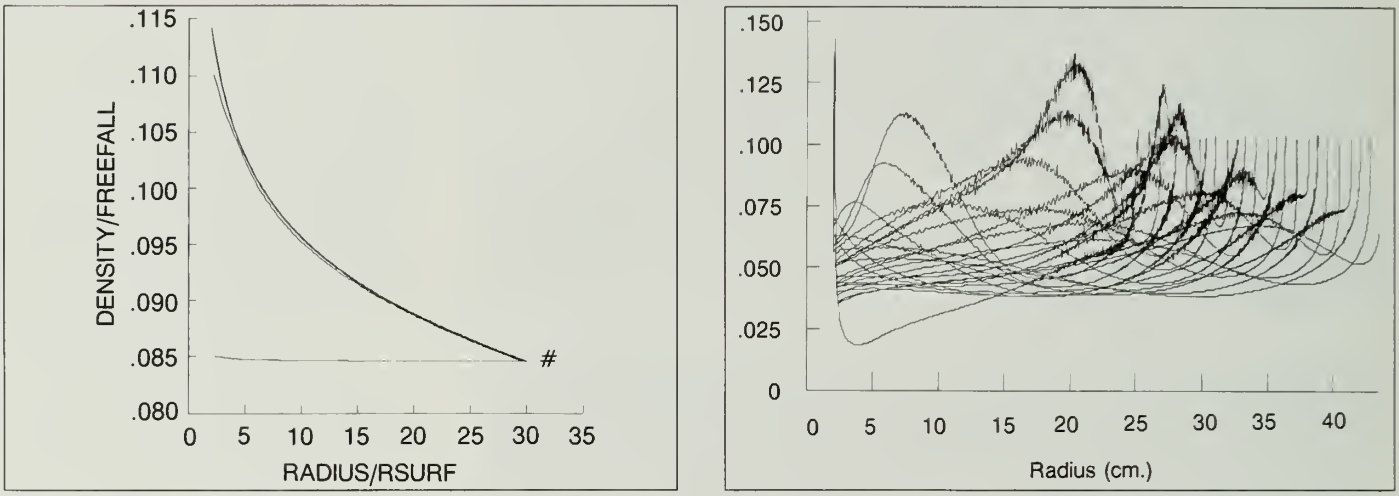
"Excellent choices, outstanding people...one of the most enjoyable and informative I've ever attended. The pace was right for me, too."

"Excellent job. Many thanks to John Larson and organizers."

"I come away from the conference with a greater appreciation for parallel processing than I had previously. I see the need to involve faculty at our university in parallel processing."

NCSA–Apple cooperate to advance science

by Ann Stowell, Product Coordinator, and Joseph Hardin, Manager, Software Development Group



Traditional plots. Density of accreting materials at various radii and points in time: (left) system settled to a particular solution; (right) system did not settle to a particular solution. (Courtesy NCSA SDG).

Months of planning and preparation within NCSA's Software Development Group (SDG) have culminated in a unique opportunity for NCSA and scientists from all over the nation to display the results of their work. Apple Computer Inc. is making a CD ROM containing NCSA's Scientific Visualization Software Suite, as well as nearly 300 Mbytes of scientific images generated by researchers who have used the software suite and other NCSA software. [For further information about the NCSA Scientific Visualization Software Suite, see page 14.] Sciences that will be represented on the CD range from fluid mechanics to cardiology. In addition to NCSA software and images, the CD will contain *Mathematica* notebooks and planetary images generated at NASA.

Rob Wolff, senior research scientist in the User Technologies Group at Apple, has been collaborating with NCSA's Software Development Group to prepare the Apple Science '89 CD. According to Dr. Wolff, Apple intends the CD "to provide students and researchers access to a high-quality sampling of scientific images and animations." Apple hopes that the CD will instruct students and researchers in the art of image-processing of numerical simulations. The CD will be particularly beneficial for those who do not have large-capacity disks of their own. It will be distributed free of charge at this summer's SIGGRAPH convention in Boston, MA and at numerous universities across the nation.

Images and better science

Scientists from a variety of research institutions around the country have submitted images for the Apple Science '89 CD to demonstrate their work and the effectiveness of the NCSA Scientific Visualization Software Suite.

Brand Fortner, scientific liaison at NCSA and a doctoral candidate in astrophysics at UIUC, exemplifies how the software suite is changing the way scientists analyze the results of their research. He reports how the software suite recently helped him analyze a particular type of X-ray oscillation observed in some binary star systems. According to Mr. Fortner, astrophysicists have been puzzled by the mysterious "sloppy periodicity" apparent in X-ray observations of a few systems that are assumed to contain neutron stars. Because the oscillation is not fixed or regular, as variations linked to regular orbits or rotations would be, this periodicity could not be explained by variation in orbits or rotations.

So, Mr. Fortner and Dr. Guy Miller, postdoctoral research associate in the UIUC Department of Physics, performed a time-dependent numerical simulation of a neutron star accumulating material from a companion star. The model was developed by Professor Fred Lamb, also of the UIUC Department of Physics. Early numerical results of the simulation were one-dimensional, and traditional methods of analysis provided little insight into the problem.

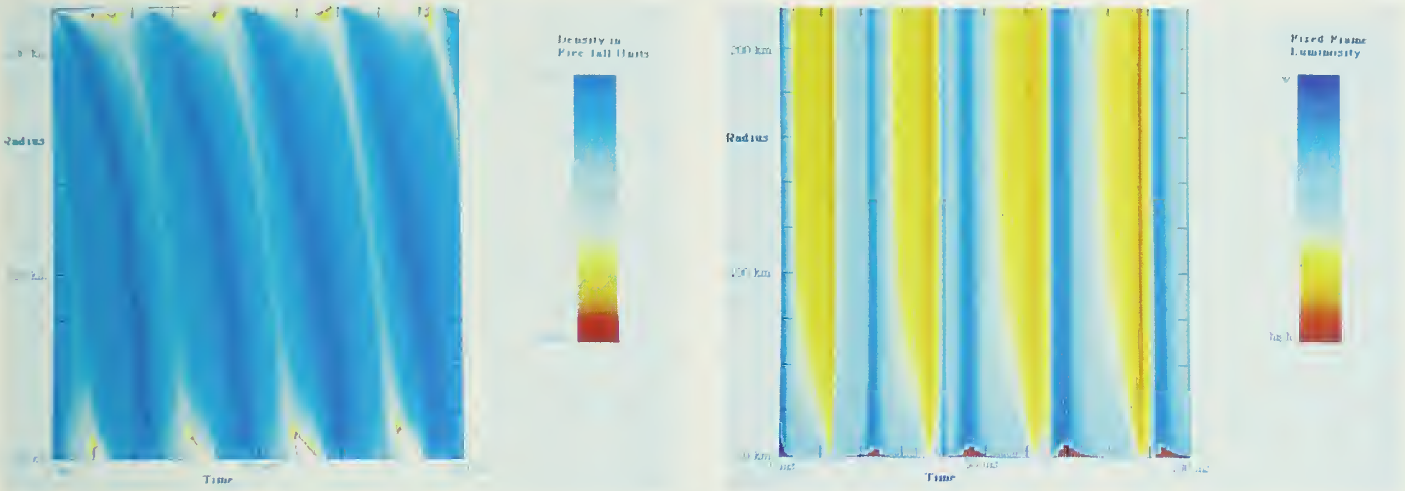
Mr. Fortner gathered results at numerous times during various simulations—plotting the radial distance from the neutron star along the x axis and the density of accreting material in grams per cubic centimeter along the y axis. In some simulations, the system settled down to a particular solution making the graph easy to interpret (see left, page 12). But when a number of times were plotted for a simulation run that did not settle down to a particular solution, the resulting graph was essentially unintelligible (see right, page 12).

Solving the mystery

To unveil the mystery obscuring the periodicity of a neutron star's luminosity, Mr. Fortner used NCSA's Scientific Visualization Software Suite. He input each density/radius profile at a particular simulation time into a two-dimensional Hierarchical Data Format (HDF) array, which he created by incorporating a single HDF subroutine call in the Cray Fortran simulation program. Each column in this HDF array is equivalent to a single line from the plot shown on the right, page 12. A column in the HDF array represents the same radius and density values for a particular point in time as a corresponding line in the original plot. In each column, radius values are represented along the y axis, and density is represented by color values. By allowing color to be incorporated as an additional variable and aligning the columns consecutively along the y axis, the structure of the HDF array made it possible to clearly represent the behavior of the star system over time.

Using the FTP capabilities of NCSA Telnet, Mr. Fortner transported the resulting dataset to his Macintosh where he could immediately load it into NCSA DataScope and NCSA Image. In NCSA DataScope, he was able to display the HDF array as a two-dimensional color raster image that represented the density of accreting material at various radii over time. The resulting image revealed a clear pattern in the results, whereas the same information displayed in a conventional graph had only compounded confusion (compare left above, page 13 and right opposite, page 12).

Because this pattern was made evident, Mr. Fortner was able to note that parabolas on the image reflected the movement of masses of material. He calls these masses "blobs." When such a blob falls onto a neutron star, where surface gravity is about 200,000 times that on Earth, it produces a burst of X-rays. Mr. Fortner theorized that the radiation pressure of the X-rays caused by this burst impedes the accretion of material onto the star, permitting new blobs to build up at the boundary of the star. When the luminosity decreases, the cycle is repeated. Specifically, the decrease of radiation pressure allows blobs to fall full-force onto the star, causing another eruption.



Software suite plots. (Left) density of accreting material at various radii over time; (right) luminosity over time (Courtesy NCSA SDG).

Getting quick answers

NCSA DataScope enabled Mr. Fortner to test this theory in a matter of minutes. With a single menu command, he generated another image, which represented luminosity over time (see right above). Using NCSA DataScope's synchronized selection capabilities, Mr. Fortner was able to select a region of high density in the first image and confirm that the corresponding luminosity in the second image revealed an increase in intensity at the moment of impact—as he had predicted.

By loading his images into NCSA Image, Mr. Fortner was able to manipulate the palette to verify his model of the observed X-ray periodicity. More importantly, he was able to

Cooperate *continued on page 16*

NCSA's Scientific Visualization Software Suite

by Ann Stowell, Product Coordinator, and Joseph Hardin, Manager, Software Development Group

NCSA's Software Development Group designed the Scientific Visualization Software Suite to provide a complementary environment for data analysis and imaging. The suite is comprised of six tools for the Macintosh: NCSA Telnet, NCSA HDF, NCSA Image, NCSA DataScope, NCSA PalEdit, and NCSA Layout.

NCSA Telnet and NCSA HDF make data transfer across great distances and between diverse machines a quick, simple, and efficient process. The copy and paste capabilities of the Macintosh and the HDF format provide a basis for the cooperative, interactive nature of the other tools. For example, you can calculate a new scientific dataset in NCSA DataScope; transfer it into NCSA Image for imaging analyses and experimentation; use a palette tailored specifically for the purpose in NCSA PalEdit; and annotate the resulting images, palettes, and data in NCSA Layout to create effective, presentation-quality slides and photographs.

See page 16 for further information about how to obtain NCSA software.

NCSA Telnet is the Macintosh's link to the TCP/IP networks. It is an implementation of DARPA standard telnet and provides interactive access from any Macintosh to telnet hosts on TCP/IP networks. NCSA Telnet lets you have simultaneous connections to numerous computers across the network. It includes a standard file transfer server (FTP) to allow you to share files with other remote machines and users. Moreover, NCSA Telnet includes VT102 emulation; Tektronix 4014 emulation; color raster graphics capabilities; domain name lookup; user-defined macro keys; full-color, font-style, and font-size support; and customized windows whose contents may be scrolled, cut, copied, pasted, and printed.

NCSA HDF, or Hierarchical Data Format, is a multi-object file format designed to facilitate the transfer of graphical and floating-point data between various machines and operating systems, including the Cray, Sun, Alliant, Silicon Graphics, Macintosh, and IBM PC computers. The format allows self-definition of data content and easy extensibility for future enhancements or compatibility with other standard formats. NCSA HDF includes Fortran and C calling interfaces; utilities to prepare raw image or data files for use with other NCSA software; an interface for storing and retrieving compressed or uncompressed raster images with palettes; and an interface for storing and retrieving scientific datasets of up to seven dimensions together with information about the data, such as labels, units, formats, and scales for all dimensions.

NCSA Image is a color-imaging application that displays and animates 8-bit binary scientific data stored in raw raster or HDF files. NCSA Image produces color raster images according to a user-defined or built-in palette. It generates black-and-white contour, ordered dither, shaded data, and three-dimensional plots. It lets you plot linear selections of data in an XY graph, perform histogram color adjustments on raster images, and print any of the black-and-white plots. Moreover, NCSA Image allows you to rotate, compress, or expand colors within the active color palette and to view actual floating-point numbers.

NCSA DataScope is an interactive data analysis tool that displays 32-bit floating-point scientific data values in spreadsheet form. In NCSA DataScope, you can represent a dataset as any of three color raster images—simple scaled, interpolated, or polar. NCSA DataScope allows you to find the data values that correspond to points on the images and to derive new datasets from your scientific data by entering analytic equations in a special notebook window. NCSA DataScope contains a wide variety of built-in functions and lets you incorporate any number of functions contained in external libraries. In addition, NCSA DataScope records and saves your observations and comments in the notebook window.

NCSA PalEdit allows you to interactively create customized color palettes, or color lookup table resources. With NCSA PalEdit, you can modify the whole palette or individual entries in a palette to produce a "clut" resource tailored to your needs. The colors in your palette can be composed of any combination of color components from four color models—RGB, CMY, HSV, and HSL. Moreover, NCSA PalEdit lets you copy and save your palettes, so that they can be pasted from the Clipboard or read from HDF files into other applications.

NCSA Layout helps you convey the results of your investigations and analyses in a professional form. It allows you to display and annotate two-dimensional data images so that you can photograph your Macintosh screen display with a 35mm camera and produce presentation-quality slides. Your layout may include several images annotated with grid lines and tick marks; text; color bars that display the range of the current palette; graphics from non-NCSA software such as MacDraw, PowerPoint, and PixelPaint; and a colored canvas. By loading or pasting user-defined color palettes into NCSA Layout, you may vary the appearance of the images and the color of your text and canvas. You can save a layout as an HDF file that may be edited at a later date; or you can save any part of a layout as a raster image that may be transferred to other machines or programs for photographing, animation, or display. ▲

New X Window packages

by Ann Stowell, Product Coordinator, and Dave Thompson, X Project Leader, Software Development Group

Two new scientific software packages released for beta test by NCSA's Software Development Group (SDG) this July demonstrate SDG's efforts to equip a wide range of systems with quality visualization software. The new tools, NCSA X Image and NCSA X DataSlice, were designed for the X Window System, an environment SDG expects to become increasingly popular.

The X Window System

The X Window System was developed by MIT in 1984. It is a network-based graphics window system whose client-server architecture allows you to run an X application on one machine (the client), while the program displays on another (the display server). For example, you can run NCSA X Image or NCSA X DataSlice on the system that stores your data, such as the CRAY X–MP/48 or CRAY-2 supercomputer, and control and view the application from your remote Macintosh, IBM RT, Sun Workstation, or any other machine that supports color X Windows.

The X platform gives the illusion that your local machine has much greater CPU power than it truly has. In the words of Dave Thompson, SDG's X project leader, "It is like having a Cray CPU board in your Mac." Moreover, the structure of the X Window System eliminates the hassles involved with data transfer across systems. These factors combine to make X software tools, such as NCSA X Image and NCSA X DataSlice, ideally suited for scientific projects that involve the Cray computers or other high-powered computer systems.

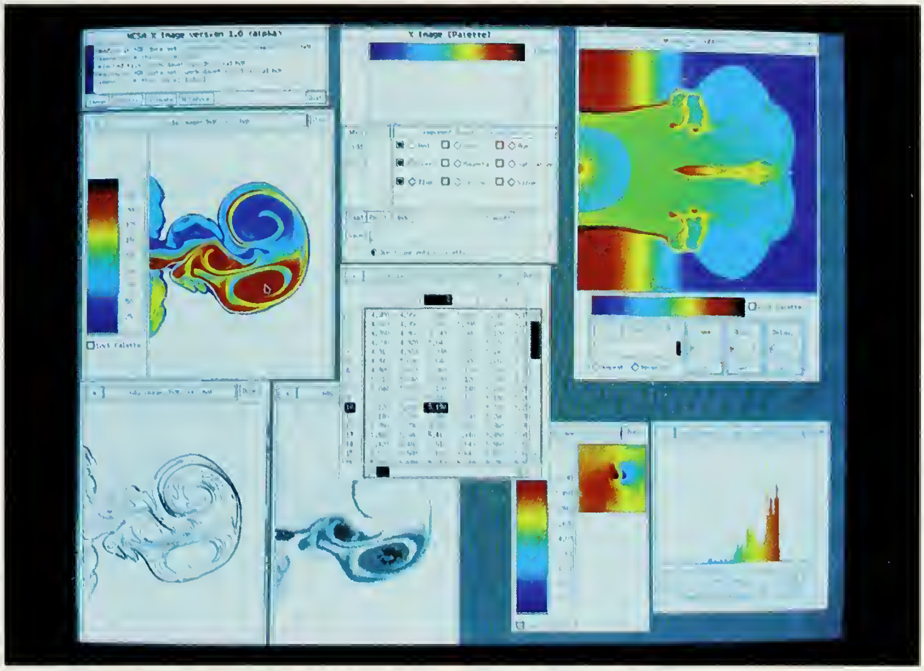
NOTE: Cray Research Inc. plans to release the latest version of the X Window System (X11R3) with UNICOS 5.0 to be installed on the NCSA Cray systems in September 1989.

NCSA X Image

NCSA X Image combines much of the functionality of the recently released Macintosh tools: NCSA DataScope, NCSA Image, and NCSA PalEdit. The application reads HDF (Hierarchical Data Format) and raster 8-bit images, as well as two- and three-dimensional HDF scientific floating-point datasets.

NCSA X Image provides a comfortable mouse- and button-driven interface. With a single click of the mouse button, you can display a dataset as real data values in spreadsheet form, a Cartesian or polar color raster image, or a contour or shaded data plot. The program permits contour and shaded overlay of raster images as well as pixel or bilinear interpolation expansions and compressions, and animation of multiple color raster images.

NCSA X Image allows you to determine which colors are mapped to your real data values. You can compose palette colors using individual components from any of three color models—RGB, CMY, and HSV. Or you can perform holistic operations such as rotating, flipping, smoothing, or "fiddling" the palette. NCSA X Image updates the color table as you manipulate the palette so that your changes are immediately reflected in the image.



NCSA X Image (Courtesy NCSA SDG).

Like NCSA DataScope, NCSA X Image lets you scroll through your actual datasets and find the values that correspond to points on associated images. Moreover, it can evaluate mathematical expressions, permitting you to apply analytical equations to your data to derive new datasets.

NCSA X DataSlice

NCSA X DataSlice was developed to permit scientific analysis of three-dimensional datasets. The application reads three-dimensional, floating-point, scientific datasets stored in HDF files. Using NCSA X DataSlice, you can view and analyze any two-dimensional plane of data along the three Cartesian coordinate x, y, and z axes as actual numeric values and color raster images. When you select a range of data values or points in an

X Windows *continued on page 16*

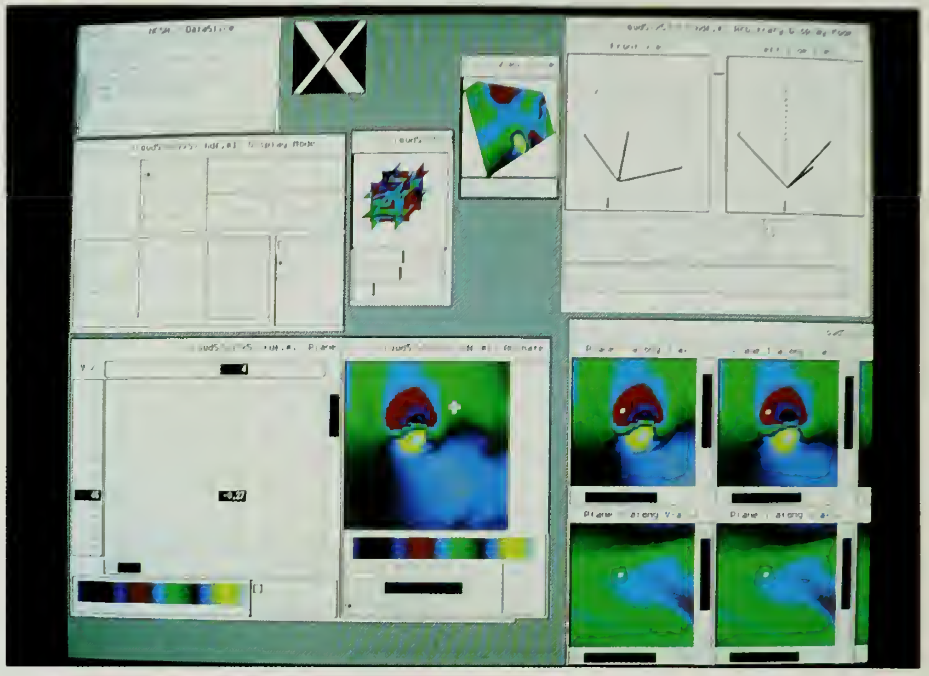
X Windows continued from page 15

image, respectively, NCSA X DataSlice highlights the corresponding selection in the image or dataset. Images generated by NCSA X DataSlice are displayed in 8-bit color, and palettes stored in either raw raster or HDF format may be used to initialize the hardware color table.

NCSA X DataSlice provides numerous ways to dissect and analyze a three-dimensional dataset. For example, you can:

- tile in a single image window several two-dimensional data slices sequentially obtained from along a single axis. (Selections in these images are synchronized, so that selecting a point in one image highlights the corresponding point in the other images.)
- "unfold" each box of data obtained from sequential planes, so that the xy, xz, and yz planes are displayed simultaneously.
- arbitrarily select and view two-dimensional data slices of any angle in the three-dimensional dataset.
- incorporate time as a third dimension and animate two-dimensional slices along any coordinate axes. (NCSA X DataSlice's animation feature allows continuous and single-step progression, manual frame control, frame skipping, auto-reverse, and asynchronous discontinuation.)
- interpolate the generated images. (A bilinear interpolation is performed for planes along the axes, and a trilinear function for arbitrary planes.)

The latest version of NCSA X DataSlice contains a three-dimensional visible volume renderer that lets you view the three-dimensional dataset as a whole and select and view surfaces within a three-dimensional scientific dataset by setting opacity transfer functions. ▲



NCSA X DataSlice (Courtesy NCSA SDG).

How to obtain NCSA's public domain software

You may obtain NCSA software by downloading if you are connected to Internet or you may order it through the accompanying *Technical Resources Catalog*.

How to download

If you are connected to Internet (NSFNET, ARPANET, MILNET, etc.) you can download software, documentation, and source code if it is available, at no charge from an anonymous file transfer protocol (FTP) server at NCSA. The procedures to do so are presented in the *Technical Resources Catalog*. If you have any questions regarding the connection or the procedure, consult your local system administration or network expert.

How to order

To order this or other software developed at NCSA, see the accompanying *Technical Resources Catalog*. Order forms are included in the publication. If you want to receive additional copies of the catalog, contact the NCSA receptionist at (217) 244-0072.

Cooperate *continued from page 13*

plot horizontal selections from the first image in an x-y plot and thereby analyze the densities of matter at particular radii for all points in time.

When asked to explain the impact of the NCSA Scientific Visualization Software Suite on his work, Mr. Fortner told this story. "On Sunday night we started to use HDF for our visualization. Within half an hour, I had the dataset in NCSA DataScope, and we made our discovery. On Monday morning, we loaded the results into NCSA Layout, created our displays [two of which are shown on page 13], and photographed our Macintosh monitor. By that afternoon, we had full-color slides suitable for a presentation to be given the following day by Dr. Miller."

According to Mr. Fortner, this discovery might never have been made without the software suite. "The research simply would not have been possible without these sorts of tools," he says. Mr. Fortner's datasets, images, and the NCSA Layout presentations he and his collaborators constructed will be featured on the Apple '89 CD. ▲

NCSA–Apple Mac IIx equipment grant program

by Fran Bond, Technical Editor

Apple Computer Inc. recently granted approximately $830,000 in equipment and funds to NCSA for support to hardware and software research and development in computational science and engineering. The grant included 62 Macintosh IIx fully configured systems and 6 LaserWriters valued at $640,000 and R&D funds totaling $190,000. According to Peter Zukowski, technology projects manager of Apple's External Research–Advanced Technology Group, NCSA's Mac IIx Equipment Grant Program is one of Apple's largest donations to date.

Two aspects of the grant are unique—the arrangement is with a laboratory at a university and the terms of the contract are less stringent than usual. Mr. Zukowski states that Apple has donated equipment to 150 universities, and this is one of the largest equipment grants that has been given to a university laboratory.

Program features

According to Mary DeLay-Goodstein of NCSA's Industrial Program, the purpose of the grant is to support several of the center's research endeavors and to promote the Mac IIx as a scientific workstation. Because of this donation, Mac IIx systems are being used for various research interests: computational superthrusts, scientific research projects, advanced computational technologies, faculty collaborative projects, NCSA Visitors Program, Software Development Group projects, Computational Science and Education Program projects, scientific administration systems integration, and high-school level mathematics education at University High School in Urbana, IL.

As part of the equipment grant requirements, sixty-two recipients will prepare quarterly reports on their research accomplishments in exchange for the use of the machines.

Each recipient of a Mac IIx also must let Apple use, modify, and create derivations from any software, hardware, or prototype that stems from research on the equipment. Apple will be able to display any prototypes developed with the equipment (NCSA will share these rights). Users also must acknowledge the grant support in their research publications.

Eligibility to participate in the program is extended to NCSA staff members or member groups; adjunct faculty, visiting faculty, or academic researchers at UIUC; and select remote research affiliates engaged in R&D.

Since NCSA participated in the prerelease testing of the Mac IIx, the center is particularly excited about this equipment grant. According to Joseph Hardin, manager of the Software Development Group (SDG), NCSA was a "seed" site for the Mac IIx motherboard, or field-upgradable version of the new 68030 (IIx) board. SDG used it to test out NCSA-developed software. This also enabled SDG's staff to learn the system's peculiarities early and give feedback to Apple.

Enthusiastic participants

Ms. DeLay-Goodstein, who is managing the grant agreement with Apple, says that there were more applicants who wanted to participate in the program than there were computers.

She says that the grant recipients are extremely enthusiastic about their computers and the results on their projects to date. For example, at University High School where the Mac IIx was introduced for teaching precalculus and calculus this past spring, students lined up to use the Mac. The students were very excited about using *Mathematica* on the Mac as a tool to learn the foundations of calculus.

A variety of other disciplines are using Mac IIxs in their research. These include: scientific research institute administration systems integration; electrical engineering (visualization of solid state semiconductor simulation); biomedical sciences (research, workstation development, record system development, and imaging); physical sciences (numerical general relativity, three-dimensional numerical thunderstorm modeling, application software and code development for astrophysical fluid dynamics); education (development of interactive lectures in higher mathematics and development of an interactive teaching environment in simple linear and nonlinear differential equations); and computer science (software development of applications and productivity tools customized for computational scientists' needs and visualization of the performance of multiprocessor operating systems).

Mac IIx and medical education

Eager medical students and residents from the College of Medicine utilize one Mac IIx 24 hours a day at Mercy Hospital, a MEDnet site. MEDnet is an innovative, multidisciplinary program for health care professionals [see ***access,*** January–February 1989]. Dr. David P. Lawrance is assistant director of MEDnet and principal investigator of its Undergraduate Medical Education Project. He is an assistant professor of internal medicine at UIC's College of Medicine at Urbana-Champaign. Dr. Lawrance reported as follows:

> Of the six Macintosh IIxs which were granted to seed MEDnet at NCSA, one was placed with a LaserWriter in the Clinical Education Center (CEC) at Mercy Hospital [in Urbana, IL]. We fondly refer to it as 'Wolffie' in honor of Rob Wolff [senior scientist at Apple]. ...The CEC is the hub of undergraduate clinical education at the hospital. ...Most of our students are combined M.D.–Ph.D. students and therefore are usually computer literate. The Macintosh has been in almost constant use since its installation.
>
> The foci of activity are computer-based education, medical records support, and transfer of NCSA visualization software into a clinical setting. Without even an introduction to the residents and students, they are now using the Mac to maintain patient logs, to write up their histories and physicals—just the sorts of things that I had expected they would use the MS-DOS computer for three years ago.

Mac IIx *continued on page 18*

***Mac IIx** continued from page 17*

The challenge is to both integrate the Mac into clinical teaching and to interest faculty in using it. Several years ago, I would have thought faculty involvement to be the inpenetrable problem, but so many of our students own their own Macs (and love using a IIx) that they sell the "Wolffie" for me.

. . . . . .

My research is in clinical image processing, and it has been an absolute delight to be able to directly transfer my images into NCSA Image. The NCSA suite of Image, DataScope, PalEdit, and Layout fit beautifully into our clinical educational environment.

. . . .

I have used it [the Mac IIx] to compose a series of medical images to be used with NCSA Image, hopefully to be included on a CD ROM which NCSA and Apple are producing [see page 12 of this issue]. Included are a few examples of color micrographs, a pseudocolored magnetic resonance image, and an animation sequence of an actual echocardiogram.

Other grant recipients were equally pleased with using the Mac IIx in their research says Ms. DeLay-Goodstein. Because space is limited, their reports could not be included.

Software development

Apple gave NCSA an unrestricted grant for the development of software for the Mac IIx and module, or component, applications. Ms. DeLay-Goodstein says Apple sees NCSA as a "frontier pusher" due to its part in the development of many innovative Macintosh II software tools, such as NCSA Image [see ***access***, March–April 1989].

The RIVERS Project (Research on Interactive Visual EnviRonmentS), an interdisciplinary effort to investigate, prototype, and develop a system that supports interactive visualization and simulation, also received funding [see ***access***, May–June 1988]. Apple will benefit from this project as information is exchanged with NCSA.

System configuration

All the workstations donated by Apple are fully configured. Basic hardware configurations for each workstation are:

- Mac IIx HD 80/4Mbyte CPU
- Apple extended keyboard
- Mac video card expansion kit
- Apple color hi-res RGB monitor
- Mac II video card
- Apple EtherNet card
- Apple monitor stand

NCSA–Apple staff support

The NCSA Workstation Systems Group is responsible for maintenance support and operating system updates. Ginger Winckler is manager of the group. Other contacts for NCSA include: Joseph Hardin, manager of the Software Development Group; Bob Haber, director of the RIVERS project; and Michael Welge, acting manager of the Applications Software Group.

Along with Mr. Zukowski, the contacts at Apple include Barbara Bowen, manager of External Research; Rob Wolff, senior scientist; Julie Lieber, research coordinator; Larry Tesler, vice-president of Advanced Technology; and David Nagel, director of User Technologies.

Emphasizing that NCSA's diverse scientific environment naturally lends itself to this collaboration with Apple, NCSA Deputy Director Jim Bottum says, "Our role is integrating the Mac into the scientific computing environment. NCSA is an excellent facilitator." He adds, "We are fortunate to have Mary here to help us with strategic vendor relationships. This area is so vital to our future and has grown so much that we needed someone with Mary's background to concentrate on it for NCSA." ▲

Second annual User Group Meeting

by Janice Knapp-Cordes, Assistant Training Coordinator

The second annual NCSA User Group Meeting will be held at the Beckman Institute (BI) on October 23–24, 1989. A new feature of this year's meeting will be the tutorials that are to be held following the meeting on October 24–25.

The purpose of the Users' Group Meeting is to foster communication. NCSA staff members will be talking about the changes and growth of the last year and outlining the plans for the next year. The users will be bringing their experiences, questions, problems, and suggestions to discuss. Each presentation will have time for questions and answers. At the end of the first day, there will be feedback and discussion groups. Speakers and many staff members will be available for informal discussion throughout the meeting. And Jim Bottum, deputy director for Operations, Planning, and Client Relations, will facilitate an hour-long question and answer period on the second day.

The User Group Meeting will open with vendor exhibits and a wine and cheese reception at University Inn which is providing accommodations for out-of-town visitors. A complete set of documentation will be available for study, and workstations will also be available for use. The conference dinner will feature a keynote address by Professor John Kogut, UIUC Department of Physics, who is one of the longest-term users of NCSA.

In response to requests from users, tutorials have been scheduled to follow the User Group Meeting. The first tutorial, a hands-on workshop on the suite of software tools developed by NCSA's Software Development Group, will be held on Tuesday afternoon from 3:00 to 5:00 p.m. Wednesday's tutorials will include UNICOS Shell Scripts and Selected Utilities in the morning and Autotasking in the afternoon.

A letter of invitation to the User Group Meeting, the agenda, and the registration form are included as inserts in this issue of ***access***. Please take a moment to look through the agenda. If you have concerns or suggestions for the agenda, please contact Janice Knapp-Cordes by phone at (217) 333-0085 or by electronic mail at janicek@ncsa.uiuc.edu (Internet) or 13036@ncsavms (BITNET).

Serving our user community is of the utmost importance to NCSA. We can best do this with your input. We hope as many of you as possible will join us in October to help us shape the future of NCSA. ▲

Fourth Summer Institute

by Phil Hattwick, Student Technical Editor

This year's summer institute participants were treated to a star-studded seminar—one that included lectures from Jack Worlton of Worlton and Associates and Los Alamos National Laboratory; Stephen Wolfram of Wolfram Research Inc. and UIUC Department of Physics; Tony Warnock of Los Alamos National Laboratory; and Karl Hess of the Beckman Institute, the Semiconductor Physics Group, and UIUC Department of Electrical and Computer Engineering.

Twenty-eight graduate students and faculty and seven industrial researchers attending NCSA's fourth annual Summer Institute (June 19–30) spent two weeks at NCSA learning about NCSA's research environment and testing that knowledge during lab sessions.

Alan Craig, NCSA graphics consultant who coordinated the program, said the institute taught students "How to use the NCSA systems, how to speed up their codes, how to use new (research) techniques such as viewing data visually through computational graphics, and how other scientists are using supercomputers in their research." He said the overall goal was "to educate graduate students and faculty in computational science and supercomputing" and show what lies in the future for supercomputers and research.

Topics included UNICOS usage and UNICOS script writing; programming tools (timing tools, editors, debuggers); vectorization and optimization; algorithm selection; math libraries; graphics software; workstation tools; and multitasking. Some of the special presentations included an overview of *Mathematica* by its designer, Stephen Wolfram; scientific visualization at NCSA; workstation futures; alternate architectures; numerical algorithms; and the Research on Interactive Visual EnviRonmentS (RIVERS) project at NCSA.

Jack Worlton, lifetime laboratory fellow of Los Alamos National Laboratory and president of Worlton and Associates—a consulting firm specializing in supercomputing, spoke on "Trends in Supercomputing." He described and analyzed forecasting methodology and made some prognostications for the 1990s. Dr. Worlton said that while the rate at which supercomputers are getting bigger and better may later slow down somewhat, it will be full speed ahead for some time now. He predicted the use of supercomputers and massively parallel computers as complementary resources—even on the same code. "I don't know what language I will be using in the 1990s," he stated. "But I know what it will be called—Fortran." He explained that while Fortran started out as a language for serial machines, it keeps evolving to accommodate new architectures.

During free hours, participants had time to interact with various NCSA staff. At a dinner during the institute, Kurt Schmucker of Apple Computer Inc. demonstrated new visualization tools soon to be released for Apple's Macintosh line. Participants also had access to NCSA workstations day and night so they could explore the systems on their own.

"The attendees will hopefully take the knowledge they've gained and go help other people at their own institutions," Mr. Craig said.

Students, faculty, or researchers from the following institutions attended the institute:

Amoco Corporation
Clemson University
FMC Corporation
Illinois Institute of Technology
Jet Propulsion Lab
Motorola, Incorporated
Northwestern University Medical School
Sampson Technical Consultants
Southern Illinois University
S.U.N.Y. at Buffalo
Texas A&M University
University of California–Santa Barbara
University of California–Santa Cruz
University of Colorado
University of Houston
University of Illinois–Chicago
University of Illinois–Urbana-Champaign
University of Massachusetts
University of Missouri–Kansas City
University of Notre Dame
University of Wisconsin–Madison
Washington State University

Jack Worlton.

Funding for the 1989 Summer Institute was provided by NCSA's Industrial Program, Cray Research, Inc., and NCSA. For further information, contact Alan Craig, graphics consultant. ▲

Selected upcoming meetings

13th Conference on the Numerical Simulation of Plasmas
September 17–20
Hilton Hotel, Santa Fe, NM.
For more information, contact Mike Norman, member of Scientific Organizing Committee, at (217) 244-2006.

NCSA User Group Meeting
October 23–24
NCSA, Beckman Institute, Urbana, IL. For more information, contact Janice Knapp-Cordes, assistant training coordinator, at (217) 333-0085.

June Peer Review Board meeting

by Patricia Wenzel, Manager, User Administration

NCSA encourages you to apply for time on the supercomputers; cycles are available on both the CRAY X-MP/48 and CRAY-2 systems.

The PRB meets quarterly in September, December, March, and June of each year. Application deadlines are the first of the month prior to the meeting.

The joint NCSA/Pittsburgh Supercomputing Center Peer Review Board met on June 20 at Pittsburgh, PA. Two new board members had been added since the last meeting: John Hawley, Astrophysics, University of Virginia; and Ahmed Sameh, Computer Science, University of Illinois at Urbana-Champaign. This was the second busiest meeting in the board's history: 51 proposals were reviewed representing requests of 29,410 service units.

Nine proposals were for multiyear requests, reflecting the board's willingness to alleviate the need to write a full proposal every year. The board did stipulate that the out-years of multiyear requests would be granted based on review of a progress report and the availability of computing cycles.

NCSA principal investigators and their approved projects

David R. Andersen, University of Iowa, *Proposal to Investigate Three-Dimensional Self-Bending of Asymmetric Optical Beams in Nonlinear Refractive Kerr Media*, CRAY X-MP/48 and CRAY-2, 150 SUs.

Won Ho Choe, University of Illinois at Urbana-Champaign, *Laser-Driven Ultrastrong Magnetic Pulse Generator*, CRAY X-MP/48, 150 SUs.

Haldan N. Cohn, Indiana University, *Dynamical Evolution of Globular Clusters and Galactic Nuclei*, CRAY X-MP/48, 200 SUs.

Antony R. Crofts, University of Illinois at Urbana-Champaign, *Prediction of Protein Structure from Sequence*, CRAY-2, 5 SUs.

Donald E. Ellis, Northwestern University, *Optical and Conductive Properties of Stacked Macrocyclic Polymers*, CRAY-2, 95 SUs.

David Ernst, Texas A & M University, *Hamiltonian Lattice Gauge Theory and Pion-Nucleus Collision*, CRAY X-MP/48, 200 SUs.

Scott Kahn, University of Illinois at Urbana-Champaign, *Modeling Quinone Reductases*, CRAY-2, 250 SUs.

J. A. McCammon, University of Houston, *Theory of Biomolecular Structure and Dynamics*, CRAY X-MP/48, 3600 SUs (3 years).

Michael Norman, University of Illinois at Urbana-Champaign, *Numerical Simulations of Radio Galaxies in Cluster Environments*, CRAY X-MP/48 and CRAY-2, 3271 SUs (3 years).

Volker Oberacker, Vanderbilt University, *Microscopic Heavy Ion Theory*, CRAY-2, 200 SUs.

Yoshitsugo Oono, University of Illinois at Urbana-Champaign, *Large-Scale Cell Dynamics of 3-D Spinodal Decomposition*, CRAY-2, 330 SUs.

Jean E. Osburn, Naval Research Laboratory, *Electronic Structure Calculations for Mn doped TiA1*, CRAY-2, 100 SUs.

V. R. Pandharipande, University of Illinois at Urbana-Champaign, *Monte Carlo Studies of Heavy Nuclei*, CRAY-2, 500 SUs.

Klaus Schulten, University of Illinois at Urbana-Champaign, *Molecular Dynamics Simulations of the Reactions at the Ubiquinone Binding Site of the Photosynthetic Reaction Center of* Rhodopseudomonas Viridis and *Molecular Dynamics Study of the Primary and Secondary Electron Transfer in a Photosynthetic Reaction Center*, CRAY-2, 630 SUs.

June PRB: NCSA allocation statistics

Number of NCSA proposals	**26**
CRAY X-MP only	5
CRAY-2 only	17
CRAY X-MP and CRAY 2	4
Fully allocated	10
Partially allocated	8
Deferred	5
Not allocated	3

	X-MP	**CRAY-2**	**Both**
Hours requested*	2293	5282	2041
Percent allocated^	76%	53%	95%

* These figures reflect what is allocated for the coming year only. They do not include service units for years two and three of multiyear requests.

^ Some allocations were deferred pending requests for additional information from researchers. These will be acted on prior to the next board meeting. Deferred allocations are not included in these figures.

Larry Smarr, University of Illinois at Urbana-Champaign, *Vacuum Geometrodynamics*, CRAY X-MP/48 and CRAY-2, 1200 SUs (2 years).

Brian Thomas, University of Illinois at Urbana-Champaign, *Fluid Flow and Heat Flow Modeling of Continuous Casting*, CRAY X-MP/48 and CRAY-2, 100 SUs.

Jack Waite, Jr., Southwest Research Institute, *Saturn Aeronomy Model*, CRAY-2, 50 SUs.

Andrew H. J. Wang, University of Illinois at Urbana-Champaign, *Interaction of Nucleic Acids with Solvent and Ligands*, CRAY-2, 100 SUs.

Peter Wolynes, University of Illinois at Urbana-Champaign, *Non-Equilibrium Statistical Mechanics Tertiary Structure Recognition Using Associative Memory Polymer Hamiltonians*, CRAY-2, 500 SUs. ▲

Renewed funding from NSF

by Jim Bottum, Deputy Director, Operations, Planning, and Client Relations

The National Science Board, the policy arm of the National Science Foundation, has approved the continuation of the NCSA Cooperative Agreement from FY91 through FY95. NCSA's total funding package is $76 million for the five-year period, which represents a more than 75 percent increase over the first five years' funding. NSF has targeted the additional funding for specific activities, including supercomputer and mass storage upgrades, remodeling, space, and staff.

In addition, NCSA is eligible to apply for "flexibility funds" targeted for activities for the center which are not basic services. This could include software development, support for alternative architectures, post docs, visitors, and so forth.

NCSA logo wins award

by Jarrett S. Cohen
Public Information Specialist

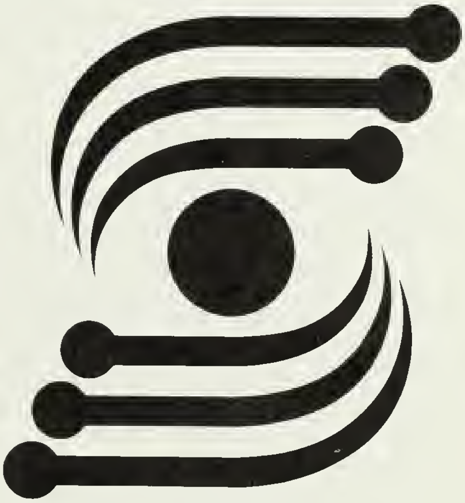
NCSA's logo will be featured in the fifth annual edition of the *American Corporate Identity*, which "shows the best in United States design," says company chairman David E. Carter. It is one of 700 winners chosen from 3,000 entries throughout the country.

"It was a very nice surprise for me," said Roman Duszek, designer of the logo. He called NCSA's visual identity program the most complex he has done in the US. Now an associate professor of graphic arts at Southwest Missouri State University in Springfield, he was a visiting professor of graphic design in the College of Fine and Applied Arts at UIUC when he designed the logo.

A native of Poland, Professor Duszek has received over twenty awards for his design work. For instance, his logo for Lot Air (the Polish national airline) won an international Corporate Identity Program prize, for which only ten designers were invited to compete. His numerical system for orientation in cities was honored by the ICSID (International Council of Societies of Industrial Design). ICSID, which groups design organizations from around the world, is based in Kyoto, Japan.

Logos are judged by Mr. Carter and two designers chosen from around the nation. Other winners in the American Corporate Identity competition include Burson-Marsteller of Chicago, McDermott Design of St. Louis, Primo Angeli of San Francisco, and Milton Glaser Inc. and The Pushpin Group of New York City.

The American Corporate Identity/5, a hardbound book of more than 100 pages in process color, is published by the Art Direction Book Company of New York City. The book is distributed worldwide and many design firms buy it, says Mr. Carter. According to him, "It is a major reference work." ▲



New and updated online information

by Will Ridenour, Online Documentation Editor

There is a new branch on the online help tree called calendar which will contain scheduled NCSA events of interest to users. Among the types of information it will contain are:

- Downtime schedules
- Backups (and purges) for user systems
- Training dates
- Peer Review Board meetings
- Visits to remote sites
- Consulting office schedule
- Conferences
- Other important dates for allocations

The following online man pages and help files have been added or updated as of June 12, 1989:

UNICOS man pages

NOTE: An ^{x} means that the man page (and the software it refers to) is currently available only on the CRAY X-MP/48.

Name	Description
abaqus	Finite element analysis package
amber^x	Macromolecular modeling package
ampac^x	Semi-empirical molecular orbital analysis package
ansys^x	Finite element analysis package
cadpac^X	Ab initio molecular orbital analysis package
charmm21^X	Macromolecular modeling package
chemistry	Overview of chemistry application packages
ds	Reports free disk space on file systems
ellpack	Solves elliptic partial differential equations
gamess	Ab initio molecular orbital analysis package
gaussian86^X	Ab initio molecular orbital analysis package
gprlsa^X	General protein least squares analysis package
mm2	Semi-empirical molecular orbital analysis package
mopac	Semi-empirical molecular orbital analysis package
pisces	Two-carrier, two-dimensional semiconductor device modeling program
ranfold	Predicts significance of RNA structures
rnafold	Folds RNA sequences
space	Reports free disk space on scratch and home file systems
suprem	Process modeling program for semiconductor devices

To view a man page, enter: `man` ***`manpage`***

where manpage is the name of the man page you wish to read.

UNICOS help files

Topic Name	Description
access	Network addresses for NCSA supercomputers are under the following subtopic: machines
calendar	The latest list of scheduled NCSA events. The following subtopics have been added: applications, consulting-office, downtime holidays, outreach-visits, peer-review-board small-allocation-committee, summer-institute, training
contacts	The following subtopics contain new or updated names, addresses, and phone numbers of NCSA contacts: accounts, affiliates, chemistry-user-group cray-operations, document-orders, industrial-program network, parallel-processing, receptionist relativity-mailing-list, software-coordinators, software-development user-services, visitors
software	An updated list of available and planned applications on NCSA supercomputers is available under this topic.

To view a help file, enter: `help` ***`topic`***

where topic is the area about which you want information. ▲

Recent personnel changes

Dr. **Karl-Heinz Winkler** joined NCSA as deputy director for Science, Technology, and Education in mid-July. **Jim Bottum** has become deputy director for Operations, Planning, and Client Relations. Dr. Winkler comes to NCSA from Los Alamos National Laboratory where he was director of the Numerical Laboratory. He will be a professor in the UIUC Departments of Aeronautical and Astronautical Engineering, Mechanical and Industrial Engineering, and Physics.

Brand Fortner, formerly manager of the Applications Software Group, is now an NCSA scientific liaison. He is responsible for the NCSA collaborative programs and superthrust areas at UIUC and the Beckman Institute; he is also exploring new areas for scientific collaboration with external organizations. **Michael Welge** is acting manager of the Applications Software Group.

Alan Craig, formerly manager of Training, is now active in the development and delivery of graphics training and education as a graphics consultant. As manager of Training, Mr. Craig expanded the training effort to one that has become a well-respected program which has gained national recognition. After taking on the Academic Affiliates Program in May 1988, Mr. Craig developed it into an equally successful program that gained national attention and expanded NCSA's services to affiliates. **Nora Sabelli** is the acting manager of Training; she continues as coordinator of Education. ▲

US Senator Gore proposes digital "Interstate System"

by Charles Catlett, Manager, Networking

Senator Albert Gore, Jr. (center) conducts a press conference from the NCSA Machine Room just prior to the Illinois presidential primary election, spring 1988. Behind Senator Gore (left to right) are NCSA Director Larry Smarr; Albert Gore, Sr.; and Mrs. Albert Gore, Jr. Senator Gore was one of a number of presidental candidates to visit NCSA during the 1988 campaign (Credit: Photo by The Champaign-Urbana News-Gazette).

Some 35 years ago, United States Senator Albert Gore, Sr. proposed a national highway system which would allow convenient travel throughout the US and stimulate economic growth. At the time, this notion had few supporters. After all, there were many fine, adequately surfaced roads throughout the country that made it possible to travel to literally every city and town. Today few would disagree that the billions of dollars spent on the Interstate Highway System were a strategic investment in the future of the US.

Senator Albert Gore, Jr. (D–Tenn.) has proposed a similar project—a digital, fiber-optic interstate highway system. Senator Gore has stated before Congress that he envisions "a national computer network linking academic researchers and industry, clustering research centers and businesses around network interchanges, and using the nation's vast databanks as the raw material for increasing industrial productivity and creating new products. Today, we have the ability to create an information 'Interstate Highway' for the 1990's... ."

Gore's bill before Congress

In a bill now before Congress, Senator Gore proposes a $1.7 billion program in which government would work with private industry to build a fiber-optic computer network that would run at over three billion bits per second (3 Gbits/sec)—roughly 2000 times the speed of the T1 lines used on today's NSFNET—within 15 years.

The proposed fiber-optic network, which would carry data as pulses of light rather than the traditional electrical signaling methods used on wires, is part of a more general bill that addresses hardware, software, research and development, networking, and a range of computing issues. The bill also promotes collaboration between universities, industry, and federal agencies. ▲

Motorola produces videotape from customized simulation program

by Scott Piette, Industrial Consultant, Industrial Program

Motorola Inc. recently produced a videotape that shows the electric fields created by electrical signals traveling between components on the surface of a circuit board. This project was accomplished by utilizing some NCSA-developed software and the production services of NCSA's Scientific Media Services (SMS). As they view the videotape, Motorola's circuit engineers will be able to see how the frequency and strength of a signal relate to the electric field.

By watching electric fields around circuit traces, problem areas can be identified where the electric field generated from one trace can induce a signal on an adjacent trace. When this happens, it is called *cross talk*. Using computer simulations to model the circuit boards, Motorola will be able to reduce the time required to take a circuit from prototype to production. At the same time, the noise immunity of the circuits can be improved.

Developing the simulation program

Recently Motorola developed through UIUC a specific finite-difference program that simulates the propagation of electric and magnetic fields in a multi-layered circuit board. The simulation generates two-dimensional ASCII output files containing floating-point numbers in a matrix form. There is one matrix for each step in the simulation. All of the timesteps are then combined into one output file.

Motorola's ultimate goal is to have the ability to generate videotape animations from their simulations quickly and efficiently.

A simple C program was written to read in the simulation output file, calculate the minimum and maximum values for the dataset, separate the set of numbers for each step, and write out a header with all of the numbers into an individual file for each step in the simulation. These individual files are in the format required to generate images using the Load Text option in NCSA DataScope software on the Macintosh. Once all of the files have been generated, they are downloaded to the Macintosh. By using the Macintosh and NCSA DataScope, the ASCII files can be generated into NCSA HDF, or Hierarchical Data Format, image files [see ***access***, March–April 1989]. (For further information about NCSA DataScope, see page 14 of this issue.)

Since animations generally run at 30 frames per second, 15 seconds of animation would require 450 frames. It would be a very tedious task to generate 450 frames using the Load Text option on the Macintosh. Therefore, an image generation utility was developed to run on the Cray supercomputer to generate Motorola's images by using subroutines from the source code to NCSA DataScope. The resulting code can read and interpret a text file in the Load Text format. Then using command line options, one can generate an output file with any combination of raster images, floating-point scientific datasets, and a color palette. Since Motorola began this project, SDG has written a utility called fp_to_hdf that will now do this.

Previewing the animation

To preview the animated sequence, one out of every ten images was moved to the Macintosh. Using NCSA Image, the image files were animated and adjustments were made to the colors. The last task to do before the production of the videotape was to generate titles and graphics describing the simulation. Diagrams of the surface being simulated and the input waveform were drawn using MacDraw II on the Macintosh. These drawings were cut out of MacDraw II and pasted into NCSA Layout. Once in NCSA Layout, other information was added and the output was saved into an HDF image file.

Text titles can also be generated using NCSA Layout. Once all of the extra information has been generated, additional HDF image files can be transferred to the Cray supercomputer where the rest of the animation files are stored.

SMS's role

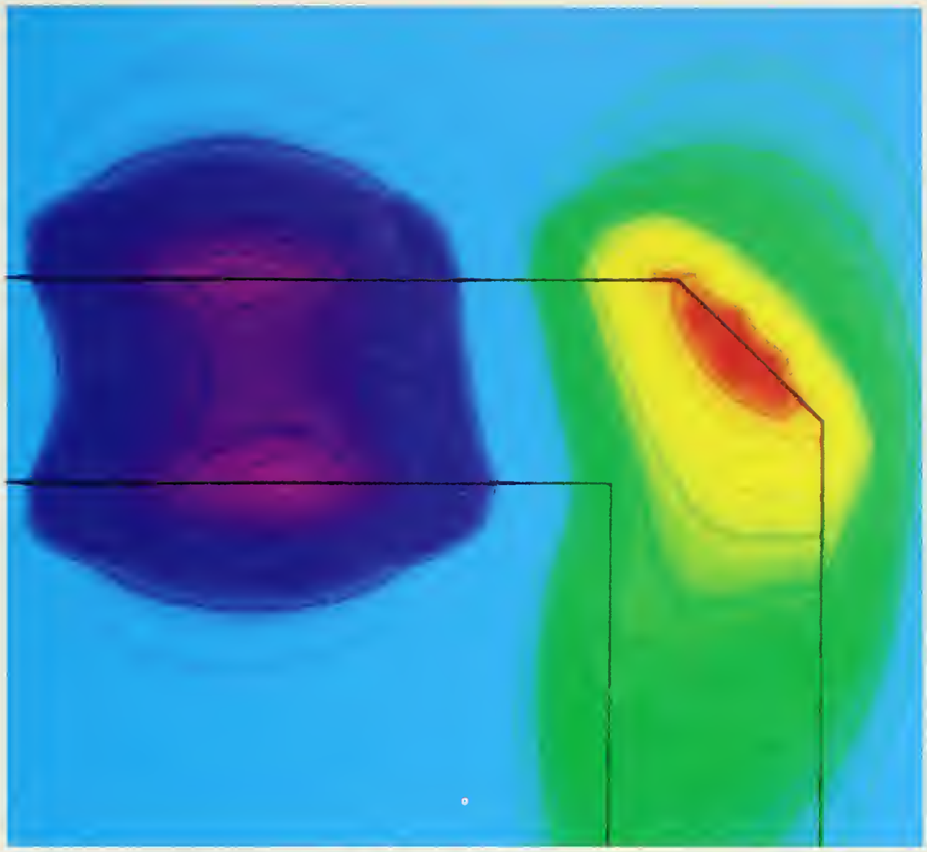
The last step after all the frames had been generated was to put the image files in the order in which they were to be animated and to assign a display rate to each frame. Scientific Media Services (SMS) can handle image files in HDF format with one image per file. The palette can be included in the HDF file with the image, but a RAW palette (not HDF palette) must be included separately with the images. SMS reserves the use of the first color (color 0) in the palette to be the background and suggests that it not be used in the image. All of the images need to be suffixed in numerical order, that is image .0001 comes before image .0002, and so forth. Then put the titles in the sequence and generate a log of the order and content of the image frames. SMS will need this information along with information on the palettes to be used with each frame, the time for the animation of the frames, what type of output is desired (that is, VHS or 3/4" U-matic), and the quantity of the videotapes to be made. All the images can be combined, along with the description file, into a tar file and put into the common file system (CFS).

When all the files were on CFS, Motorola contacted SMS and described where the files were and how they could be accessed. By working with SMS and with a little practice, Motorola was able to get an idea of the proper speed for the animation. Within a few days after the simulation had been compiled, they a complete videotape with titles, graphics, and animated simulation output was ready for presentation.

For further information

NCSA DataScope, NCSA HDF, and NCSA Layout are products of the NCSA Software Development Group (SDG). For more information on HDF files or the NCSA Macintosh utilities, contact Joseph Hardin, manager of the Software Development Group (see **NCSA Contacts**, page 28), or NCSA's Software Development Group by electronic mail at softdev@ncsa.uiuc.edu (Internet).

For questions regarding this project, contact Scott Piette, NCSA Industrial Consultant, by electronic mail at spiette@ncsa.uiuc.edu (Internet) or 13042@ncsavms (BITNET). For information about having videotapes made, contact Vincent Jurgens, coordinator of SMS, by electronic mail at vjurgens@ncsa.uiuc.edu (Internet). ▲



Right An electric field generated from a 3 GHz sine wave introduced onto the circuit board from the left side. The circuit board trace is outlined in black. The field strength ranges from red to violet showing positive field strength and negative field strength respectively (Courtesy Motorola).

Chemistry Users *continued from page 5*

calculations using the "Direct SCF" method and for more recent work of a similar nature with Möller-Plesset (MP) calculations (a type of perturbation theory) by a "Direct MP2" method.

A basic assumption is that established physical models are valid for larger molecules. Conventional methods, with some modifications, are applied to systems of nonconventional size. Currently, CPU power is less of a limiting factor than is disk capacity and I/O data transfer rate. For example, a calculation with 300 basis functions can generate a billion integrals! Thus, it is important to identify the "most computationally expensive" integrals and keep them in memory or on disk. The remaining integrals will be recomputed as needed.

Unnecessary computation can be avoided by screening 2-index exchange integrals before calculating 4-index integrals. In addition to small integrals, integrals which are not small—but also not important to the Fock matrix—can be ignored.

The "n^4 myth"

For small chemical systems, the number of integrals to be calculated increases as n^4, where n is the number of basis functions. For large systems on the other hand, integral evaluation time is proportional to n^2, not n^4, because only two-center coulomb interactions are significant.

The Direct SCF method of recalculating integrals avoids the usual disk I/O bottleneck by recalculating integrals as needed. Although this may use more CPU time, prescreening of integrals can be made efficient, point group symmetry can be exploited with less overhead, and basis set contractions are sufficiently less critical so that they may be omitted. Also, this method lends itself to easy implementation in a parallel, multiprocessor computational environment.

In discussing methods which go beyond Hartree-Fock methods, a basic electronic structure technique, Professor Almlöf touched on Möller-Plesset perturbation methods. He compared the computational capacities of a personal computer and a supercomputer for Direct MP2 calculations.

Applications and tour of BI

Professor Almlöf finished his presentation by listing several applications of interest. Among these were large two-dimensional and three-dimensional carbon clusters via Direct SCF or In-Core SCF, metal clusters via state-averaged SCF, large basis sets for small molecules, and stacking of large polymeric aromatic hydrocarbons via Direct MP2.

Refreshments and socializing concluded the meeting. Those present toured the Beckman Institute to see representative office, laboratory, and support facilities.

Interested in computational chemistry?

For further information about NCSA's Computational Chemistry Group and its iniative, contact Dr. Harrell Sellers (see ***NCSA Contacts***, page 28 and ***access***, May–June 1988). For information about software availability or to request future announcements of NCSA Computational Chemistry User Group activities, contact Dr. Joe Golab (see ***access***, March–April 1988). ▲

Latest NCSA training trips

by Alan Craig, Graphics Consultant

NCSA Training has been on the move again. NCSA consultants have been visiting remote sites to give training classes, work with researchers, and meet with computing center personnel to enable NCSA users at remote campuses to learn the latest in supercomputing.

Short summaries of some recent outreach follows:

May 22-25 Rick Kufrin, systems consultant, and Ilhan Dilber, industrial consultant, visited the campus of the University of California at Santa Barbara (UCSB). Their visit was hosted by Stefan Boeriu, the NCSA affiliate contact at UCSB. The purpose of the trip was to hold training classes and to work with individual research groups on their concerns. Training topics included UNICOS, CFT77, timing tools, NCSA policies, NQS, optimization, multitasking, and an overview of NCSA's graphics. One of the research groups that NCSA's consultants met with from the Department of Chemistry consisted of experienced users of GAUSSIAN86 under CTSS, but they were newcomers to UNICOS. Consequently, there were many questions and explanations. During their stay, Mr. Kufrin and Dr. Dilber visited the Institute of Theoretical Physics (ITP), where they met with Richard Stark and Ben Cohen to discuss NCSA software developments and their use on the two Cray supercomputers and also talk about ITP's systems.

May 3-5 Two representatives from NCSA—Sam Milosevich, industrial consultant, and Alan Craig, then manager of Training—attended the NORTHWESTNET training conference at the University of Washington in Seattle. The first day was a "preday" to the workshop. NCSA gave a course on how to use the UNICOS operating system on a remote supercomputer. Participants had the opportunity to log onto NCSA's CRAY-2 and try some lab exercises from the training room in Seattle. On the last day of the conference, NCSA gave general presentations about supercomputing and scientific visualization. Participants met with the NCSA representatives to discuss their research. Once again, participants had a chance to try the NCSA CRAY-2 as well as NCSA Image for the Macintosh, an imaging tool developed by the Software Development Group.

April 24–25 Two NCSA consultants, Rick Kufrin and Mike Krogh, gave classes to researchers at the University of Colorado at Boulder on the use of NCSA's systems and software. Specifically, course topics included UNICOS, CFT77, NQS, cdbx, multitasking, timing tools, and scientific visualization. In addition, they worked with research groups in aerospace, mechanical, and civil engineering to help them work on their codes on the UNICOS operating system.

April 6 Alan Craig, then manager of Training, and Jim Ferguson, industrial consultant, made a trip to Rose-Hulman Institute of Technology, a largely undergraduate engineering school in Terre Haute, IN. The day was spent meeting with faculty and administrators. NCSA's representatives discussed the options available to help Rose-Hulman incorporate supercomputing into their undergraduate engineering curricula and the possibilities for networking. The highlight of the day was a presentation by NCSA to a group of about 70 undergraduate students about supercomputing, computational science, and scientific visualization. After the talk, there was a demonstration of the NCSA Software Development Group's new software suite for the Macintosh (for details, see page 14 of this issue).

To arrange for NCSA representatives to visit your campus, contact the Coordinator of the Affiliates Program [see **NCSA Contacts**, page 28]. ▲

Educational outreach to Augustana

by Alan Craig, Graphics Consultant

Dr. Nora Sabelli, coordinator of Education, and Alan Craig, then manager of Training, visited Augustana College in Rock Island, IL in April. Augustana, a primarily undergraduate institution, recently became a member of the NCSA Affiliates Program.

One purpose of the trip was to welcome Augustana as an NCSA affiliate institution and provide training for a number of the faculty. Training consisted of an introduction to the use of NCSA's Cray systems and an explanation of the policies and procedures for using NCSA. There was a lab session in which faculty had the opportunity to log on to the NCSA Cray systems and do some exercises. Everyone logged on, changed his/her password, and experimented with the system a little.

Dr. Sabelli held a presentation/discussion with faculty about how to incorporate supercomputing and computational science concepts into the courses they teach. Augustana has been chosen as a pilot school to work with NCSA on developing and using university course materials in supercomputing and computational science.

Augustana called a press conference to explain what it means to have become an NCSA affiliate. Mr. Craig demonstrated NCSA Image for the press. NCSA Image, a tool developed by NCSA's Software Development Group, allows a researcher to display, modify, and animate computer images on his/her own computer workstation.

The trip was hosted by Dr. Robert Frank, professor of physics at Augustana. Other Augustana departments represented included chemistry, computer science, and mathematics.

All in all, the day was a valuable exchange of information between Augustana faculty and NCSA staff. One result of the visit was the inclusion of Cray system exercises in the curriculum of a computer mathematics course for high school students run by Augustana in June 1989.

If your institution is interested in being visited by NCSA staff, please contact the Coordinator of the Affiliates Program, [see **NCSA Contacts**, page 28]. ▲

Training sessions

Upcoming NCSA training sessions are planned as follows:

1989	
Sept. 25–28	New User Training
Oct. 23–24	**User Group Meeting** (see page 18)
Nov. 6–10	Affiliates Training
Dec. 11–14	New User Training

General

Fortran 8x forwarded for second public review

by Kurt Hirchert, Systems Consultant

At its May meeting, X3J3, the committee responsible for the ANSI Fortran standard, completed work on a revision of its proposed Fortran 8x standard and voted to forward it for a second period of public comment. At the same meeting, X3J3 also completed work on its official responses to the comments received during the first public comment period.

Several of the more complicated features of the original draft have been simplified or eliminated in the revised draft, but several new features—most notably a pointer facility—have been added in response to the public comment. This draft remains controversial. One camp argues that Fortran must be significantly enhanced in order to adequately support the scientific and engineering computing community in the next decade and that the costs of supporting such an enhanced language are manageable and acceptable. Another group argues that (1) these costs will be so great as to destroy the properties of Fortran that have made it popular with the scientific and engineering community and (2) that applications which cannot be adequately supported by Fortran should be migrated to some other language.

The second public comment period is scheduled to run from July 27 through November 24, 1989. During this period, comments may be sent to:

Public Comment for dpANS Fortran Revision
Attention: Lynn Barra
X3J3 Secretariat
311 First Street NW, Suite 500
Washington, DC 20001-2178

If you are interested in what Fortran will look like a decade from now, you are strongly encouraged to participate in this second public review.

Copies of the Fortran 8x draft can be obtained from Global Engineering Documents by phoning 1-800-854-7179. If you are outside the United States, you may find it convenient to obtain the ISO version of this document through your national standards body. Or if you wish to order from Global Engineering Documents, contact their international sales representative, Mike Ozmun, at (714) 261-1455 or use their FAX number, 1-714-261-7892.

NCSA systems consultant Kurt Hirchert is a member of X3J3. He would be happy to answer questions about the revised draft or otherwise assist you in the public comment period. Contact him at (217) 333-8093. ▲

History of Fortran

Fortran was originally developed three decades ago by a team at IBM. In 1966, it became the first computer language to be standardized. In 1978, a revision of that standard was approved. This revision, popularly known as Fortran 77, included many features that were already widely implemented. It also included features, such as the CHARACTER data type and the block-IF construct, that were not a part of most existing Fortran implementations.

During the public comment period for Fortran 77, X3J3 received many suggestions that it felt were reasonable but could not be incorporated into that standard without unduly delaying its adoption. Instead, it agreed to consider those suggestions for inclusion in the next revision of Fortran. Shortly after the adoption of Fortran 77, X3J3 surveyed various user groups to determine what features were felt to be needed beyond those in Fortran 77. It then began refining and developing those features which were most widely felt to be needed. The current Fortran 8x draft is an outgrowth of that process, although in some cases the features that resulted from this process may look significantly different from those that were originally requested. ▲

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data link Preview

- Notes and quick tips
- Hot topics in the NCSA Consulting Office
- Changes in the Network Queueing System
- Fortran 8x summary
- NCSA computational chemistry applications software
- MSC/NASTRAN version 65C available on the NCSA CRAY X-MP system
- NCAR GKS output to the IBM-3800
- ACM algorithms available to NCSA users
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Special Report

NCSA impacts science at SIGGRAPH '89

by Jarrett S. Cohen,
Public Information Specialist

From information infrastructure to thunderstorm animation, NCSA played a major role in the Association for Computing Machinery's SIGGRAPH '89 computer graphics conference July 31–August 4 in Boston, MA. A highlight of the conference was a televisualization-by-satellite demonstration.

NCSA was involved in many conference activities, including press conferences, coproduction of a compact disc, the Computer Graphics Theater, papers and panels, SIGGRAPH Board of Directors and planning committees, slide sets, and the Animation Screening Room.

Shrinking the miles

One of the major barriers to the effective use of supercomputing and visualization tools is distance. Often, as adequate network connections do not exist, NCSA users must come to Champaign-Urbana to take full advantage of the center's resources.

A few months ago, Bob Haber, head of NCSA's RIVERS (Research on Interactive Visualization EnviRonmentS) Project and associate professor of theoretical and applied mechanics at UIUC, came up with a way to solve this problem.

Bringing together the visualization and supercomputing resources of NCSA with the video technology of Sun Microsystems Inc. and a satellite link provided by American Telephone & Telegraph Co. (AT&T), Haber and his colleagues demonstrated that scientists can perform real-time interactive visualization from a remote site and collaborate over great distances as well. The televisualization-by-satellite demonstration took place at the SIGGRAPH '89 papers and panels reception Thursday evening (August 3) in the Boston Museum of Science.

SIGGRAPH continued on page 3

Supermap of the Milky Way Galaxy's center shown in the televisualization-by-satellite demo at SIGGRAPH by NCSA Research Scientist Mike Norman and NCSA postdoctoral research associate Bob Sault. Data collected and processed by Neil Killeen, UIUC postdoctoral research associate in astronomy, and Professor Fred Lo, UIUC Department of Astronomy.

Karl-Heinz Winkler is NCSA's newest deputy director... *see "Karl-Heinz Winkler's new approaches to science," page 8.*

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Abbreviations

CRI	Cray Research Inc.
CSRD	Center for Supercomputing Research and Development
IRC	Interdisciplinary Research Center of NCSA
NCSA	National Center for Supercomputing Applications
NSF	National Science Foundation
UIC	University of Illinois at Chicago
UIUC	University of Illinois at Urbana-Champaign

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SIGGRAPH continued from page 1

Commenting on the project Haber said, “Our goal is to show how the technology used in a live news or sports broadcast can provide scientists and engineers effective access to supercomputers and their colleagues—no matter how far apart they might be.”

Scientists using a Sun Workstation in Boston interactively controlled the NCSA supercomputers and visualization systems in Illinois to produce real-time animations in two and three dimensions. AT&T’s SKYNET Video Conferencing Service beamed the animations back to Boston for display in the SunVideo window on the workstation monitor, which captures and displays live video images. The images were also projected onto a large screen for audience viewing.

The major research applications in the demonstration were:

- Radioastronomy image processing with data from NCSA’s CRAY-2 supercomputer being animated on an Ultra Network Technologies frame buffer. NCSA Research Scientist and UIUC Associate Professor of Astronomy Mike Norman coordinated this segment, which generated high-resolution “supermaps” of the Milky Way’s galactic center. He collaborated with Neil Killeen, UIUC postdoctoral research associate in astronomy, and Dr. Fred Lo, professor in the UIUC Department of Astronomy, who collected and processed the data; and Bob Sault, NCSA postdoctoral research associate in astronomy, who did the technical work.

- Dynamic crack growth and stress visualization, Haber’s research area, in which CRAY X-MP/48 supercomputer data was animated on an Alliant VFX/80 minisupercomputer. The configuration and fine-tuning of these mappings were controlled from the Sun Workstation.

- A three-dimensional thunderstorm simulation from the CRAY-2 supercomputer interactively visualized on the Alliant VFX/80 was organized by NCSA Research Scientist and UIUC Professor of Meteorology Bob Wilhelmson. The operator released tracer particles within the storm and watched the computer integrate their flow paths for real-time animation.

NCSA Director Larry Smarr (left) onstage at the televisualization with Bob Haber (center), NCSA adjunct professor, and Donna Cox (right), NCSA design and research professor.

Norman in Boston—and Wilhelmson in Champaign—conducted a video teleconference, sharing their work with one another and the SIGGRAPH audience. The SunVideo window alternated between Wilhelmson and the storm simulation.

With other companies possessing these technologies, sending materials by express mail and traveling to a colleague’s laboratory will soon no longer be the only ways to collaborate.

Haber offered one example: “A scientist in California could use interactive computer animation techniques to monitor and control a simulation of a severe storm as it runs on a supercomputer in Illinois and simultaneously discuss the results with a research partner in New York or anywhere else on the globe.”

Smarr speaks at press conferences

One of NCSA’s goals is to provide leadership on the emerging national information infrastructure, which includes a national high-speed network, scientific visualization, supercomputing, HDTV (high-definition television), and interactive television. NCSA Director Larry Smarr discussed these issues and their impact upon the computer graphics industry at large.

“Politicians cannot decide what science and technology areas to legislate on unless scientists and technologists take a leadership role in shaping the agenda,” said Smarr when introducing the SIGGRAPH ’89 conference to the press. Smarr was a member of a panel Tuesday morning (August 1) that included Thomas DeFanti (moderator) of the Electronic Visualization Laboratory at UIC, Walter Bender of the MIT Media Lab, Don Greenberg of Cornell University, John Lasseter of Pixar, and Carl Machover of Machover Associates.

Smarr spoke about the need for computer models of worldwide problems such as ozone and global warming. He then gave attendees a look at visualization projects recently completed at NCSA, including “Study of a Numerically Modeled Severe Storm” and “Computer Simulation of the Global Climatic Effects of Increased Greenhouse Gases.”

These problems, Smarr said, “cannot be attacked but through a national, and then international, network,” a subject that Smarr and

SIGGRAPH continued on page 4

***SIGGRAPH** continued from page 3*

Jim Clark, chairman and founder of Silicon Graphics Computer Systems, discussed later that afternoon in a separate press conference.

"Supercomputing only comes into its own when coupled to personal computing," Smarr said. "The idea of putting a custom-made environment on everybody's desktop *is* a revolution."

A national fiber optic data superhighway, another name for this network, would hook desktop systems and supercomputers together, allowing closer collaboration than is now possible, Smarr said. Borrowing a term from NSF, he said, "What will emerge from this is a 'national collaboratory.' "

The National High-Performance Computer Technology Act of 1989 bill, sponsored by Sen. Albert Gore, Jr. (D-Tenn.) provides for such a superhighway with transfer rates of 3 Gbps [see ***access***, July–August 1989]. Currently, NSFNET runs at 1.5 Mbps, 2000 times slower than the proposed network. If the bill is passed, this network will likely be in place by the mid 1990s, Smarr said.

Much of the public discussion of fiber optics has centered around HDTV, as eventually the network will extend to people's homes. Regarding HDTV, Clark said that it must be a digital medium, unlike Japan's traditional, analog system. "The notion of the retrofitting of broadcast television is a dead end," he said.

HDTV is only one of the services a fiber optic network will enable, but the same principles apply. "We are moving from an analog world to a completely digital, interactive world," Smarr said.

Compact disc produced with Apple

NCSA's Software Development Group and Apple Computer Inc. produced a compact disc that was distributed at the conference [see ***access***, July–August 1989]. The disc contains the NCSA Scientific Visualization Software Suite for the Macintosh (NCSA Image, NCSA DataScope, NCSA PalEdit, and NCSA Layout) [see ***access***, July–August 1989] and 300 Mbytes of digital visualization images from the center and research scientists across the country. NCSA staff demonstrated these new capabilities at the Apple booth in the SIGGRAPH exhibition.

Thunderstorm in Computer Graphics Theater

A team led by Wilhelmson and the NCSA Visualization Group collaborated on a two-minute animation entitled "Study of a Numerically Modeled Severe Storm," which was shown at the Computer Graphics Theater. It was one of only 44 projects chosen out of 328 entries.

The animation consists of five narrated sequences that show the structure of severe thunderstorms and the beneficial uses of scientific visualization. Coinvestigators include graduate research assistants Harold Brooks, Brian Jewett, and Louis Wicker and research programmer Crystal Shaw. The animators were Matthew Arrott, Mark Bajuk, Colleen Bushell, and Jeffery Yost.

SIGGRAPH board member Cox publishes paper

Donna Cox, assistant professor of the UIUC School of Art and Design and NCSA design and research professor, is on SIGGRAPH's Board of Directors and arranged public relations materials for the conference. Her paper, "The Tao of Postmodernism: Computer Art, Scientific Visualization, and Other Paradoxes," was one of the lead papers selected to appear in the SIGGRAPH/Leonardo publication *Computer Art in Context: The 1989 SIGGRAPH Art Show Catalog.*

Haber panel member

In addition Robert Haber was a member of a panel on "Effective Software Systems for Scientific Data Visualization." They discussed current problems in "bringing today's technol-

Opposite page, center. NCSA staff members in Boston coordinate the televisualization-by-satellite demo with the NCSA Urbana-Champaign contingent: (center rear to right front) Bob Sault, postdoctoral research associate in astronomy; Bob Haber, NCSA adjunct professor; Dave McNabb, research programmer; and Jeff Terstreip, research programmer. Images transmitted by satellite from NCSA (opposite page, left) were received in Boston via satellite (this page, right).

Below. Still from NCSA's animation shown at the Computer Graphics Theater, "Study of a Numerically Modeled Severe Storm."

ogy into the hands of the typical scientist." Haber talked about visualization software architecture and the efforts of the RIVERS Group in developing real-time interactive tools for visualization. He showed a new method for visualizing three-dimensional tensor fields in a recently completed videotape animation.

UIC visualization group

UIC's Electronic Visualization Laboratory (EVL), codirected by NCSA Adjunct Professors Thomas DeFanti and Daniel Sandin, was also well represented at the conference. DeFanti, Sandin, and EVL Associate Director Maxine Brown spoke in three 1-day tutorial courses. Brown was also a member of the Computer Graphics Theater Committee. A paper, "Ray Tracing Deterministic 3D Fractals," by EVL graduate student John Hart, Sandin, and Mathematics Professor Louis Kauffman was included in the technical program. Images of these fractals produced by Hart also appeared in the form of video, slides, and software. DeFanti, Sandin, Hart, and graduate student Stephan Meyers collaborated with NCSA Adjunct Professor Ellen Sandor of Illinois Institute of Technology's (ART)^n Laboratory on "Chaos/Information as Ornament/Tribute to Louis Sullivan," an autostereogram exhibited in the Art Show.

EVL is NCSA's Remote Visualization Research Group. ▲

NCSA images and simulations

SIGGRAPH slide sets

Five NCSA images appeared in SIGGRAPH slide sets, which were available for purchase at the conference. The following images appeared in the technical slide set:

- "Molecular Diffusion on Single Crystal Gold Surface Studied by STM." Research: Joseph Lyding, Jerome Hubacek, Roger Brockenbrough, UIUC. Visualization: Mark Bajuk, NCSA.
- "Microscopic NMR Chemical Shift Images." Research: Paul Lauterbur, UIUC; Marcelino Bernardo, Jr., State University of New York at Stony Brook. Visualization: Mark Bajuk, NCSA.

Three images were included in the stereoscopic 3D slide set:

- "Interaction of a Gravitational Wave with a Black Hole." Research: Larry Smarr, David Hobill, David Bernstein, NCSA. Visualization: Donna Cox, Ray Idaszak, NCSA.
- "Fractalscape." Visualization: Brian Evans, UIUC; Ray Idaszak, NCSA.
- "Papilloma Virus." Visualization: Donna Cox, NCSA; Daniel Sandin, Stephan Meyers, UIC; Ellen Sandor, IIT Institute of Design.

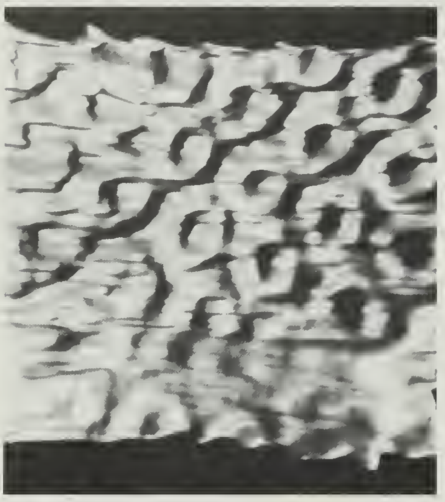
Animation Screening Room

A large number of NCSA simulations, 13 in all, were viewed in the Animation Screening Room at the Sheraton Hotel and Towers. They were also part of a series of videotapes, "Visualization/State of the Art," sold at the conference. Titles, as listed in the program, and credits are as follows:

- "The Etruscan Venus." Research: George Francis, UIUC. Visualization: Donna Cox, Ray Idaszak, NCSA.
- "Numerical Relativity: Black Hole Spacetimes." Research: Larry Smarr, David Hobill, David Bernstein, NCSA. Visualization: Donna Cox, Ray Idaszak, NCSA.
- "The Lorenz Attractor." Research: David Hobill, Michael Welge, Daniel Simkins, NCSA. Visualization: Jeffery Yost, NCSA.

***Images** continued on page 6*

Below. Images from NCSA slide sets. "Molecular Diffusion on Single Crystal Gold Surface Studied by STM" (left) and "Microscopic NMR Chemical Shift Images" (right).



- "Kodak's Supercomputational Science '88." Research: Lawrence Ray, Richard Ellson, Michael Rubinstein, Kodak; Jozef Cohen, UIUC. Visualization: Donna Cox, Ray Idaszak, NCSA.
- "Hydrogen Diffusion on a Platinum Surface." Research: Lawrence Ray, Roger Baetzold, Kodak. Visualization: Donna Cox, Ray Idaszak, NCSA; Richard Ellson, Kodak; Marc Olano, UIUC.
- "Monte Carlo Simulation of Excited Electrons in GaAs." Research: Daniel Bailey, Christopher Stanton, Karl Hess, UIUC. Visualization: Mark Bajuk, NCSA.
- "Molecular Diffusion on Crystal Gold Surface." Research: Joseph Lyding, Jerome Hubacek, Roger Brockenbrough, UIUC. Visualization: Mark Bajuk, NCSA.
- "Two-Armed Instability of a Rotating Polytropic Star." Research: Richard Dursien, Shelby Yang, Robert Grabhorn, Indiana University. Visualization: Jeffery Yost, NCSA.
- "Large-Scale Structure in the Universe." Research: R. Brent Tully, University of Hawaii. Visualization: Michelle Mercer, NCSA.
- "Enzyme Reaction in Triophosphate Isomerase." Research: Paul Bash, Martin Karplus, Harvard; Robert Davenport, MIT. Visualization: Stefen Fangmeier, NCSA.
- "Quantum Molecular Dynamics." Research: Paul Bash, Martin Field, Martin Karplus, Harvard. Visualization: Matthew Arrott, Michelle Mercer, Jeffery Yost, NCSA.
- "Cajon Pass Scientific Drilling Project." Research: Colleen Barton, Mark Zoback, Stanford. Visualization: Jeffery Yost, NCSA.
- "Topology of Coma Supercluster Region." Research: Jack Burns, University of New Mexico. Visualization: Stefen Fangmeier, NCSA.

Order information

Slide sets and videotapes may be purchased from ACM Order Department, P. O. Box 64145, Baltimore, MD 21264; phone (800) 342-6626. ▲

Below. Walid Abu-Sufah.

Supercomputing performance studies

by Kathleen Robinson, Science Writer

What makes a particular program run ten times faster on one supercomputer than on another machine of supposedly similar performance? How can an organization determine which supercomputer is the best for a particular range of applications? How should a researcher refine a code to make the best use of a particular machine? As the number of supercomputer users and manufacturers expands, such questions are becoming increasingly important.

One person working on ways to answer these questions is Walid Abu-Sufah, associate professor of computer science at Virginia Polytechnic Institute and State University, Blacksburg, VA. Abu-Sufah spent June and July at the IRC, sponsored jointly by NCSA and the Center for Supercomputing Research and Development (CSRD). In collaboration with NCSA Research Scientist John L. Larson, Abu-Sufah worked to develop a set of parameters that can be correlated with performance metrics (measurements) in a consistent fashion across different programs and, eventually, across machines.

An alumnus of UIUC, Abu-Sufah obtained his Ph.D. in electrical engineering in 1979. Prior to teaching in Virginia, he was a faculty member in the UIUC Department of Computer Science and a software engineer with CSRD. Immediately after earning his doctorate, he was on the faculty of Yarmouk University, Irbid, Jordan, where he taught electrical and computer engineering. While at Yarmouk University, he became assistant dean of engineering.

Says Abu-Sufah, "There are some very basic questions which need answers. For example, how do we measure supercomputer performance? What metrics should we use? There are no well-established techniques for evaluating supercomputer performance in a scientific manner. So our first objective is to define performance metrics. Then we want to show that there is a correlation between machine performance and characteristics of the code."

Performance tools

"We are developing tools that will enable us to measure the performance of particular programs on different machines. When a researcher says, 'My code is taking 10 hours to execute,' these tools will give us data about *why* that program is taking so long."

The first tool, Abu-Sufah explains, is for collecting data about the program during execution. "It collects data at the loop level. Current machines like those in the CRAY X-MP and CRAY Y-MP product lines give statistics about the performance of the machine at the job level or the subroutine level, but we are going inside to a smaller program segment. Parameters that people have used in the past are average vector length, how many iterations there are in a program, and the percentage of time spent in vector mode. These parameters are too macroscopic. We'd like to be more precise."

The second performance tool analyzes the assembly code produced by the compiler to examine software/hardware interactions.

Software changes

"By using these tools," predicts Abu-Sufah, "researchers may identify factors affecting the performance of their codes on particular machines. Improving that performance, then, might necessitate choosing different compiler options, rewriting parts of the programs, interchanging some of the statements—things of that sort. It might be necessary to choose different algorithms. It might even be necessary to go back to the original physical phenomenon being modeled and choose different equations for representing that."

SIAM presentation

In December 1989, Abu-Sufah and Larson will present a paper at the SIAM (Society for Industrial and Applied Mathematics) Conference on Parallel Processing in Chicago. The paper is entitled "Correlating Workload Characteristics to Performance Metrics for the CRAY X-MP/Y-MP."

In the paper, Abu-Sufah and Larson develop a methodology for defining and measuring quantitative workload characterization parameters. (Workload characterization is an integral part of computer system performance evaluation.) They show how these parameters correlate consistently with performance metrics across different programs, and they use a set of codes on the CRAY X-MP and Y-MP from different application areas to demonstrate the effectiveness of their approach. In their study, they utilize production codes from NCSA and from CSRD's Perfect Club Suite [see ***access***, May–June 1989].

> *"We are developing tools that will enable us to measure the performance of particular programs on different machines. When a researcher says, 'My code is taking 10 hours to execute,' these tools will give us data about why that program is taking so long."*

Hardware implications

Abu-Sufah says, "Eventually, these tools should be useful for generating examples for training. If they are refined even further, they could be used to identify specific bottlenecks of the hardware. We might be able to predict that a certain type of code would run faster if there were more registers, for example, or more ports to memory.

"Computer scientists have some general concepts about performance that are true most of the time, but not *all* of the time. For example, if there are more processors working on a program, we should get the answer sooner. However, that's true only up to a certain point—where the addition of more processors slows everything down. That's because of the overhead necessary to manage the different processors—the fact that they have to be managed even if they have nothing productive to do. So the concept 'Add more processors to get more performance' doesn't have a uniform correlation across the entire range. We'd like to know what the correlation is, and if it's different in different ranges, what is the cut-off point—where is the change? These are long-term possibilities. Our *first* goal is to help the user make better use of existing code." ▲

Scientific visitors

Giovanni Bachelet
September 12–27
University of Trento
Area of research: physics

Thomas Bouman
August 30, 1989–August 15, 1990
Southern Illinois University
Area of research: chemistry

Ernesto Esteban
August 30, 1989–August 15, 1990
University of Puerto Rico, Humacao
Area of research: astrophysics

John Hawley
September 29–October 1
University of Virginia
Area of research: astrophysics

L. P. Hughston
September 24–30
Robt. Fleming Securities, Ltd.,
London, England
Area of research: applied mathematics and international finance

Karl-Heinz Winkler's new approaches to science

by Stephanie Drake, Publications Editor

Above. Karl-Heinz Winkler.

"Karl-Heinz Winkler is a tremendous addition to our center. He enjoys a worldwide reputation as one of the pioneers of computational science in its broadest sense," NCSA Director Larry Smarr said when he recently introduced the new deputy director for Science, Technology, and Education to NCSA staff. He joins Jim Bottum, deputy director for Operations, Planning, and Client Relations [see ***access***, July–August 1989].

Winkler is committed to helping "establish a digital computational culture in American universities and industry." UIUC's computational reputation was the primary attraction to this numerical scientist who has spent nearly 20 years in computational science. "What is truly unique about the University of Illinois," he says, " is that for a long time computing and supercomputing have been firmly accepted as a way of doing research. Establishing a computational culture has already happened in many departments here, so NCSA is well integrated into a computational university evironment."

U.S. Senate testimony

In July—during his transition from Los Alamos National Laboratory—Winkler testified to the Senate Subcommittee on Science, Technology, and Space concerning S. 1067, the National High-Performance Computer Technology Act. This bill was introduced by Sen. Albert Gore, Jr. to provide a coordinated federal research program that will ensure continued U.S. leadership in high-performance computing [see ***access***, July–August 1989].

In his testimony Winkler stressed the need to convert from analog to digital technology and the use of computational science as a research tool. "In this culture," he said, " use of computational methods and digital exploitation of our knowledge base will be widespread and accepted as the rule, not the exception. The impact of a well-balanced national high-performance digital infrastructure will not be limited to computer scientists or to technologists but will have a positive widespread impact on all people of the United States."

He went on to explain that the current infrastructure is unbalanced in three ways: essential ingredients of an effective system are missing (in particular, large parts of existing knowledge reside only in analog form in libraries); the facilities to store large amounts of information in digital form do not yet exist; and many existing facilities cannot function to their potential because they are not fully integrated.

The current imbalance creates a negative effect on scientific research. Winkler emphasizes, "This neglect denies us a selection of computational research programs based purely on their importance. It puts undue emphasis on those programs which match the system. Thus, a well-balanced digital national infrastructure will help to produce a more balanced computational science program."

NCSA—a service center

"The world is looking at NCSA," says Winkler, and he wants the center to "lead by example."

Components of a well-balanced computational environment include computer power; large memories; communication and networking; high-speed, large-capacity data storage; data transport; visualizations to transmit information; and software to generate and extract information. The two major bottlenecks identified by Winkler are data communications and storage.

Winkler praises the accomplishments of the NSF centers program, in general; and NCSA, in particular. "The central facilities here (the Crays and mass store, for example) are excellent. And the workstations are on each researcher's desk. What's missing is an intermediate suite of hardware and software tools—such as interactive visualization, communication, and high-speed, large-capacity storage available directly to scientists—needed for many demanding scientific projects." Winkler wants to fill that gap by expanding the already successful existing suite of software tools, NCSA Scientific Visualization Software Suite [see ***access***, July–August 1989], and by extending the same homogeneous software environment across all hardware.

The major attraction of NCSA to national and international, academic and industrial researchers, according to Winkler, is that they can do things at NCSA they can't do anywhere else. Unique research will be further encouraged "by making accessible and usable a very large collection of tools and functionalities, so that our users experience a terrific gain in productivity in their work. They will be able to do things not just faster, but many difficult problems will become tractable."

Winkler is also setting up an "interdisciplinary research program" for university and industry. Looking at the sundry expertise of NCSA staff, Winkler sees that "more than a dozen scientific areas are represented on the NCSA staff." Instead of being grouped by job type (such as the former Computational Science Program), staff with different expertise but interest in similar scientific areas are now grouped into teams. A team may consist of a research scientist, an applications software specialist, a software development programmer, and specialists (consultants) in the hardware.

Winkler will lead the effort to increase the strength of existing areas—which include computational chemistry, parallel processing, finite element analysis, electrical engineering, computational astrophysics, gravity, medical imaging, mathematics and statistics, and computational fluid dynamics. He will carefully consider new areas in which to expand. Staff scientists are particularly charged with staying in touch with their scientific communities so NCSA can contribute to development within those communities.

The goal, Winkler emphasizes, is to "provide a service to the various scientific disciplines." Software development and visualization are major tools in this service to scientific communities.

The center's education program is especially concerned with providing continuing training and education for NCSA staff and to reaching out into academic and industrial communities. Winkler intends to integrate the NCSA Scientific Research Program and the Education Program with all those who are not NCSA staff—local faculty, off-campus faculty, industrial partners, and industrial and academic visitors.

"The impact of a well-balanced national high-performance digital infrastructure will not be limited to computer scientists or to technologists but will have a positive widespread impact on all people of the United States."

Numerical laboratories—a new dimension

As director of the Numerical Laboratory at Los Alamos National Laboratory, Winkler created an advanced center for interactive visualization, a laboratory that combines supercomputers with state-of-the-art graphics, storage, and networking equipment. The main emphasis of this project was to discover "how use of advanced computing technologies can increase an individual researcher's productivity."

Winkler believes that numerical laboratories, such as the one he created at Los Alamos and those he intends to create at NCSA and UIUC, are essential. Numerical laboratories provide sites to test potential new hardware and software research tools. A new tool can progress from being experimental and unreliable to becoming stable and productive. Once proven reliable in the numerical laboratory, the new software or hardware can be incorporated into the central facility and become part of the center's production service.

Numerical laboratories also offer an individual researcher working on a single scientific problem brief access to tremendous resources that are not available continually to a researcher. Users of numerical laboratories have physical access to all machinery as well as ways to enter and take out huge amounts of data. Numerical laboratories also provide a platform for vendors to integrate new products without destabilizing central facilities.

Interactive visualization is an essential tool, Winkler believes, because it provides a common language. "We can use numerical laboratories to provide theoreticians, experimentalists, and computational scientists with a common language—visualization—that will allow them to compare their insights and data. We will be able to have terrific impact on revitalizing experimental science."

A professor, too

Only a person with great energy, stamina, and mental acuity can handle the tasks Karl-Heinz Winkler has set for himself. In addition to his responsibilities to NCSA, he has also been appointed full professor in the UIUC Departments of Aeronautical and Astronautical Engineering, Mechanical and Industrial Engineering, and Physics. His first two years are committed entirely to NCSA; thereafter, his responsibilities will be divided equally among the three departments and NCSA.

To Winkler, teaching goes hand in hand with his work at NCSA—offering another means to promote and support computational science throughout the various university departments. "It is important that NCSA work even more than in the past through existing structures and contribute to building up computational science in campus departments."

Winkler *continued on page 18*

NCSA Advisory Committee meets

by Rebecca A. Pickett, Secretary, Deputy Director for Operations, Planning, and Client Relations

The NCSA Advisory Committee met in Urbana in late July. NCSA Director Larry Smarr welcomed the group and summarized events and activities that had occurred since the committee last met in December 1988 [see ***access***, January–February 1989].

Highlights of Smarr's summary are as follows:

- NCSA renewed the NCSA Cooperative Agreement for FY91–FY95 at $75 million, a substantial increase over the last funding period
- FMC Corp. signed as NCSA's fifth industrial partner in February
- Renaissance Experimental Lab is in full operation, made possible by a $680,000 equipment donation from Silicon Graphics Inc. (SGI)
- Apple Computer Inc. donated 15 Mac IIxs and $120,000 for joint NCSA–Apple software development, 6 Mac IIxs and software development funds for MEDnet, and 40 Mac IIxs for the Science Program
- Connection Machine (CM-2) provided by DARPA through NSF and installation/hook-up is in process [see page 17]
- Seminars/workshops/consultations offered 500 hours of training
- Scientific visualization made impressive strides, including a presentation of the "Big Bang Theory" for ABC-TV's "20/20" [see page 18]
- Current collaborative programs include the Center for Prokaryote Genome Analysis
- NCSA will help make history, it is hoped, with its part in the live televisualization link via satellite at SIGGRAPH '89 [see page 1]

NCSA staff members received input from the committee on the following:

- Methods of upgrading existing workstations and other equipment with a view toward creating the best overall desktop environment
- Approaches to NCSA's reorganization and space requirements necessitated by current and projected growth
- Approaches to outreach efforts, in light of proposed federal legislation that could create an enlarged national network by 1991

The Advisory Committee will meet again in December 1989. It was unanimously agreed that the December session will require two days because of the number of issues to be faced. ▲

Advisory Committee members

Ron Deiss *Chairman*
Deputy Director of NAS, NASA Ames Research Center

Ken Bishop
Professor of Petroleum Engineering,University of Kansas

Jonathan Dantzig
Associate Professor of Mechanical Engineering, UIUC

Ernest Davidson
Professor of Chemistry, Indiana University

Arthur Freeman
Professor of Physics, Northwestern University

Eric Jakobsson
Associate Professor of Bioengineering, UIUC

Lawrence Landweber
Professor of Computer Science, University of Wisconsin–Madison

Bernard O'Lear
Manager of Systems, National Center for Atmospheric Research

Jon Sauer
Adjunct Professor at Optoelectronics Computer Systems Center, University of Colorado

John Steele
Director of Computing Center, Purdue University

Robert Wolff
Senior Scientist, Advanced Technology Group, Apple Computer Inc.

Paul Woodward
Professor of Astronomy, University of Minnesota

"It's an exciting place!"

by Stephanie Drake, Publications Editor

Above. Deborah Lee.

Deborah Lee was certainly in the right place at the right time. The former director of administration and controller at Minnesota Supercomputer Center Inc. had moved to central Illinois when her husband relocated here about a year ago. Several months later she happily saw the opening for associate director for finance and administration at NCSA. The search committee was just as happy to find someone experienced in the operations of a supercomputer center to replace Harriett Weatherford, who had left to become associate vice chancellor for research at UIUC.

Lee already knew a little about NCSA: it was a Phase II NSF supercomputer center, and it had a strong interest in visualization. But she did not realize how large and successful NCSA had become.

Jim Bottum, deputy director for operations, planning, and client relations, recently introduced Ms. Lee to NCSA staff by saying,"We are very fortunate in that Debbie brings to this position both the educational background and the state university 'know-how' necessary to get the job done."

Lee identifies two primary purposes for herself and her staff of 16. On the finance side, they handle the business office, day-to-day responsibilities, and contracts; administer grants; and make certain NCSA complies with regulations. Their administrative purpose is to serve the rest of the center, thereby helping NCSA carry out its mission. Lee says that administration traditionally doesn't grow as fast as the rest of a company but is needed to provide ongoing high-quality service. She wants to build up the administrative infrastructure and to enhance and develop financial reporting procedures that will aid in planning and control for the center.

"Most things seem tame after working at a supercomputer center."

Qualified educationally for her position, Lee received a BSB–Accounting from the University of Minnesota and later earned her CPA. Before taking the position at Minnesota Supercomputer Center, Ms. Lee worked as a senior accountant for Peat Marwick Mitchell (now Peat Marwick Main). And long before she became interested in the business side of research, she did hands-on research as a technician in a university-related animal research laboratory.

It's easy to see that Ms. Lee enjoys working at NCSA. She grins when she says, "It's an exciting place! I really like being back at a center. Most things seem tame after working at a supercomputer center." ▲

Reminder: User Group Meeting

by Janice Knapp-Cordes, Assistant Training Coordinator

As this issue goes to press, final preparations are being made for the second annual NCSA User Group Meeting. The meeting's objective is to facilitate communication between users and NCSA staff and among users.

This year's meeting is being held at the Beckman Institute on Monday and Tuesday, October 23 and 24. On Sunday evening, October 22, a reception at University Inn will kick off the meeting. John Kogut, UIUC professor of physics and long-term NCSA user, will be the keynote speaker at Monday evening's dinner.

A new feature this year are tutorials on October 24 and 25, which will follow the meeting. The topics available are software development tools, UNICOS shell scripts and selected utilities, and autotasking.

For further information, contact Janice Knapp-Cordes, by telephone at (217) 333-0085 or by electronic mail at janicek@ncsa.uiuc.edu (Internet).

New software releases from NCSA

by Mary Hocks, Technical Writer, Software Development Group

The scientific software packages being released by NCSA's Software Development Group (SDG) early this fall demonstrate SDG's continuing efforts to equip a wide range of systems with quality visualization software. Two of the new tools, NCSA X Image and NCSA X DataSlice, have been designed for the X Window System, a unique environment SDG expects to become increasingly popular. Other new applications include NCSA MedImage, NCSA HyperCard Scientific Animation Package, and NCSA Height-Color Visualizer, as well as updated versions of NCSA Layout and NCSA HDF (Hierarchical Data Format).

These packages are available through anonymous file transfer protocol (FTP). See the end of this article for instructions on obtaining this software.

NCSA X Image 1.0 for the X Window System combines the functionality of the recently released Macintosh tools NCSA DataScope, NCSA Image, and NCSA PalEdit. It allows you to view and manipulate data values, including datasets calculated on the CRAY X-MP or CRAY-2 systems. The application reads HDF and SEQ raster 8-bit images, as well as two- and three-dimensional HDF scientific floating-point datasets. By clicking on a button, you can display a dataset as real data values in spreadsheet form, as full color Cartesian or polar raster images, or as a contour or shaded data plot. Image manipulation features include animation of multiple-color raster images.

NCSA X Image also allows you to determine which colors are mapped to your real data values. You can compose palette colors and perform global operations such as rotating, flipping, smoothing, or "fiddling" the palette. The application updates the color table as you manipulate the palette so that your changes are immediately reflected in the image. X Image features color histograms of the frequency distribution of data.

NCSA X DataSlice 1.0 for the X Window System was developed to permit scientific analysis of three-dimensional datasets. The application reads three-dimensional, floating-point datasets stored in HDF files. Using NCSA X DataSlice, you can view and analyze any two-dimensional plane of data along the three Cartesian coordinate axes—x, y, and z—as actual numeric values and color raster images. When you select a range of data values or points in an image, the application highlights the corresponding selection in the image or dataset. Images generated by NCSA X DataSlice are displayed in 8-bit color, and you can load user-defined palettes to enhance imaging and analysis.

NCSA X DataSlice provides numerous ways to dissect and analyze a three-dimensional dataset. For example, you can tile in a single image window several two-dimensional data slices selected along a single axis. Selections in these images can be synchronized, so that selecting a point on one image highlights the corresponding point on all other images. You can "unfold" each box of data obtained from sequential planes so that the xy, xz, and yz planes are displayed simultaneously. You can also incorporate time as a third dimension and animate two-dimensional slices along any coordinate axis. The updated version of X DataSlice contains a visible volume renderer that lets you select and view surfaces within a three-dimensional scientific dataset by setting the opacity transfer functions, light sources, texture maps, and so forth.

NCSA MedImage 1.0 for the Macintosh is a version of NCSA Image tailored specifically for medical imaging. NCSA MedImage supports vertical edge, horizontal, Sobel, Laplacian, and median kernel convolutions; image rotation and overlay; and both rank order and frequency domain filtering. It features several new analysis tools, including the protractor tool. NCSA MedImage reads two-dimensional slices of data from three-dimensional files, as well as two-dimensional datasets from several types of generic, raw data files.

NCSA HyperCard Scientific Animation Package 1.0 for the Macintosh allows you to create a movie animation of a series of graphic images simply and efficiently. It is an add-on XCMD for HyperCard that imports sequences of graphic images into a HyperCard stack. Specifically, the package allows you to translate graphic images, typically created on a Cray supercomputer and translated into a series of Tektronix 4014 drawing commands, into a PICT file; read the resultant file into a HyperCard stack; and animate the images.

NCSA Height-Color Visualizer 1.0 for SGI 4D Workstation Systems is a noninteractive batch utility that enables you to easily create three-dimensional animations from time-dependent data. Input data for the Height-Color Visualizer consists of 2 two-dimensional arrays, each having a single variable at every node. Using the Height-Color Visualizer, you can manipulate the first of the 2 arrays to create a height geometry, while the program creates a color field using the second array. When the color field is draped over the height geometry, both fields assume the same input dimensions. Thus, analyzing the correlation of data in the NCSA Height-Color Visualizer is as easy as associating regions of height with coincident regions of color.

NCSA Layout 1.2 for the Macintosh helps you present the results of your investigations and analyses in a professional form. It allows you to display and annotate two-dimensional data images so that you can photograph your Macintosh screen display with a camera and produce quality slides for presentation. Your layout may include several images annotated with grid lines and tick marks; text; color bars that display the range of the current palette; graphics from non-NCSA software such as MacDraw, PowerPoint, and PixelPaint; and a colored canvas. By loading or pasting user-defined color palettes into NCSA Layout, you may vary appearance of the images and the color of your text and canvas. You can save a layout as a raster image that may be transferred to other machines or programs for photographing, animation, or display. The newest version of NCSA Layout includes batch animation capabilities and laser printing capabilities.

NCSA HDF 3.0 is a multi-object file format designed to facilitate the transfer of graphical and floating-point data between various machines and operating systems, including the Cray, Sun, Alliant, Silicon Graphics, Macintosh, and IBM computers. The format allows self-definition of data content and easy extensibility for future enhancements or compatibility with other standard formats. NCSA HDF includes Fortran and C calling interfaces; utilities to prepare raw image or data files for use with other NCSA software; an interface for storing and retrieving compressed or uncompressed raster images with palettes; and an interface for storing and retrieving scientific datasets of up to seven dimensions together with information about the data, such as labels, units, formats, and scales for all dimensions.

The updated version of NCSA HDF includes new interfaces for palette input/output and 24-bit raster images, for storing and retrieving annotations, and for slicing datasets.

Obtaining public domain software from NCSA

You may obtain NCSA software by downloading if you are connected to Internet or you may order it through the NCSA *Technical Resources Catalog,* August 1989.

How to download

If you are connected to Internet (NSFNET, ARPANET, MILNET, etc.), you can download software, documentation, and source code if it is available, at no charge from an anonymous file transfer protocol (FTP) server at NCSA. The procedures to do so are presented in the *Technical Resources Catalog.* If you have any questions regarding the connection or the procedures, consult your local system administrator or network expert.

How to order

To order this or other software developed at NCSA, see the *Technical Resources Catalog,* August 1989. Order forms are included in the publication. If you want to receive additional copies of the catalog, contact the NCSA receptionist at (217) 244-0072. ▲

Industrial Program

Dow Chemical becomes sixth partner

by Jarrett S. Cohen, Public Information Specialist

Dow Chemical Co. has signed as the sixth partner in NCSA's Industrial Program.

A four-year, $3.3 million agreement, effective October 1, allows Dow researchers and computer experts to receive extensive training in advanced computing technologies and conduct supercomputer-based research at the Center.

"Supercomputing is a tool that in the long run will help keep us competitive in our industry, " said Irv Snyder, director of research and development for Dow. "Through this partnership, our people will be able to learn from the Center's experts about this leading edge technology."

Added Robert Nowak, director of Dow's Central Research Laboratories: "Dow's continued interest in using the newest, most sophisticated computational analysis available has led us to join the supercomputing program at NCSA. The facilities and support system at the Center was one of the determining factors in our joining this particular National Science Foundation site.

"Our interests in supercomputing are very broad, ranging from theoretical analysis of process chemistries to working with computer-aided design of molecules for use in polymers and in pharmaceutical and agricultural chemicals."

Some of the projects Dow researchers plan to pursue at the Center include modeling of compounds and reactions, reactor design, process optimization, fluid dynamics, and catalysis.

"Dow's addition reinforces one of our priorities—to enhance the development and manufacturing of chemical and plastic products," said Larry L. Smarr, director of NCSA. "I know their team and our team working together will make major advances, as NCSA believes the application of advanced computing technologies can greatly improve the competitiveness of American industry."

Based in Midland, MI, Dow Chemical is one of the world's largest producers of chemical, plastic, and specialty products for agriculture, automobiles, construction, electronics, packaging, pharmaceuticals, and consumer uses. Dow and its subsidiaries operate facilities at 158 sites in 32 countries and maintain more than 190 sales offices. In 1988 Dow's sales totaled $16.7 billion. ▲

Kodak extends its agreement

by Jarrett S. Cohen, Public Information Specialist

Eastman Kodak Co., the first industrial partner of NCSA, has extended its agreement to work with the center's supercomputers.

With the 16-month, $1.3 million extension to the original three-year, $3 million industrial supercomputing agreement, Kodak researchers and engineers will continue to receive comprehensive training in advanced computing technologies and to do supercomputer-based research at the center.

"Our experience during the last three years has demonstrated convincingly that supercomputer technology is an effective tool for theoretical, as well as applied, science," says Edwin Przybylowicz, senior vice president and director of research at Kodak. "NCSA, coupled with the interdisciplinary Beckman Institute at the University of Illinois, offers Kodak a unique opportunity to meet many of the research and engineering challenges posed by our diverse portfolio of product technologies."

Larry Brandt, associate director of the National Science Foundation's Supercomputer Centers Program, says that "Kodak's decision as NCSA's first industrial partner sends a key signal to American industry.

"At first, the idea of getting corporate involvement was something of a gamble; we did not know if using NSF funds to leverage industry support would work," Brandt says. "The center's track record with industry to date and Kodak's willingness to expend its investment in supercomputing proves that the experiment has been a decisive success."

Kodak, which had $17 billion in sales last year, in August 1986 became the first major corporation to join NCSA's Industrial Program. Since then, it has been joined by Amoco Corp., Eli Lilly and Co., Motorola Inc., FMC Corp., and Dow Chemical Co.

"I am very pleased with Kodak's extension," said Larry Smarr, NCSA director. "Our partnership has been beneficial to both of us, and I am especially pleased to see Kodak's advancements in the use of computational science."

In one project, Kodak researchers have used the UIUC supercomputing center's resources to look at diffusion mechanisms on metal surfaces. "These mechanisms are important to such processes as film development and catalytic reactions," said Larry Ray, Kodak's senior research scientist working at the center.

Based in Rochester, NY, Kodak is one of the world's leading producers of photographic products, commercial and information imaging systems, chemicals, plastics, and pharmaceuticals. Kodak has manufacturing and marketing facilities in 45 countries and employs more than 145,000 people. ▲

Education

Supercomputing education workshop

by Kathleen Robinson, Science Writer

For 12 intensive days in July, researchers and educators from across the country gathered at NCSA for the first NSF-sponsored Supercomputer Education Summer Workshop. Although most participants brought with them working code for use in lab sessions, the focus was *not* on their own research but on techniques for encouraging the use of supercomputers by their scientist colleagues and students.

Daily seminar topics plus clinics and lab sessions that often stretched far into the night were only part of the agenda. The 16 select attendees [see opposite page] prepared final presentations and also participated in group discussions that could help national centers determine the most appropriate materials and procedures for serving as educational resources to the nation's universities.

Dr. Nora Sabelli, NCSA manager of Education and Training, based the supercomputing education workshop on a 10-week workshop she developed while at UIC [see ***access***, May–June 1988]. The goal of this compressed workshop at NCSA was to enable faculty members and industry professionals in computationally intensive fields to develop similar courses or workshops at their home institutions or within their professional organizations. Sabelli believes it is necessary "to foster in all disciplines familiarity and adaptability to the advances in computer technology. Because of the rapidly changing nature of the technology, it is not logical to pursue the 'learn as you go' approach that has had to suffice in the past." It is expected that participants in the workshop will be better able to incorporate supercomputing concepts into classes they teach, into their own work, and into collaborative or consultative efforts with others.

Participant selection was based on a number of factors, including knowledge of at least one supercomputer system or of mainframe code development and a willingness to serve as a consultant or model at the home site. Disciplines represented ranged from computer science, physics, and engineering to fields not usually considered to be computational—namely, geography and music.

Access via Internet to various advanced computing architectures and operating systems enabled the workshop participants to concentrate on basic issues and concepts of supercomputing across architectures rather

Far left. Workshop coordinator Nora Sabelli. **Left.** Andrew Sung (New Mexico Technological University) gives his presentation. **Below**. Participants (left to right) Ken Bishop (University of Kansas), Marilynn Livingstone (Southern Illinois University–Edwardsville), and M. Fouad Ahmad (University of Madison–Wisconsin) discuss the day's session.

than on individual computer techniques. Computers and systems used in the workshop included the CRAY X-MP/48 and CRAY-2 supercomputers running UNICOS at NCSA and the IBM 3090 600E/VFS running CMS at the Cornell National Supercomputer Facility (CNSF).

Beginning with the November–December 1989 issue, future articles in ***access*** will focus on some of the workshop participants, their presentations, and developments in supercomputing education at their sites. ▲

Workshop personnel

Participants
Roger Abell, Arizona State University
Om Prakash Agrawal, Southern Illinois University–Carbondale
M. Fouad Ahmad, University of Wisconsin–Madison
Kenneth Bishop, University of Kansas
Hui-Ying Chung, University of Nebraska
Daniel Griffith, Syracuse University
Mahmood Haghighi, Bradley University
Xiong He, Syracuse University
Horngming Hsieh, UIUC
Chinh Le, Vanderbilt University
Marilynn Livingston, Southern Illinois University–Edwardsville
Michelle Nearon, State University of New York at Buffalo
Anthony Pearson, University of California at Santa Cruz
David Renneke, Augustana College
Andrew Sung, New Mexico Technological University
Sever Tipei, UIUC

Auditors
Amy Bug, Swarthmore College
Linda McDonald, North Park College

Speakers
Charles Catlett, NCSA
Michael Folk, NCSA
Charles Henderson, CNSF
John Larson, NCSA
Bruce Leasure, Kuck and Associates
Thomas Moher, UIC
T.J. O'Donnell, graphics consultant
David Padua, David Sehr, and Samuel Midkiff, CSRD
Tomas Putnam, Purdue University
Ann Solem, LANL

Lab consultants
Robert Fiedler, NCSA
Ramesh Jayaraman, NCSA
James Joseph, NCSA
Gary Kakazu, NCSA
Rick Kufrin, NCSA
Chip Mayse, NCSA
Satheesh Menon, NCSA
Steve Morley, NCSA
Scott Morton, NCSA
Robert Panoff, Clemson University
Stephen Roy, UIC
Nora Sabelli, NCSA
Ann Solem, LANL
Todd Saunders, NCSA

Connection Machine workshop

by Fran Bond, Technical Editor

Above. Jacek Myczkowski, scientist from Thinking Machines's home headquarters in Cambridge, MA introduces PARIS (so-called for Parallel Instruction Set), the CM-2's lower-level language. (Credit: Jack Gladin, CSL)

Participants

Representatives from the following institutions attended:

Amoco Corp.
UIUC (3)
Clemson University
Eastman Kodak Co.
FMC Corporation (2)
LANL
Michigan State University
Motorola Inc.
North Carolina State University
Pennsylvania State University
Southern Illinois University–Edwardsville
UIUC (5)

Left. Workshop participants, including Karen Diemer from LANL, work through the coffee break. (Credit: Jack Gladin, CSL)
Below. Bernie Murray (right), Thinking Machines representative from the Knowledge Representation and Natural Language Division at Chevy Chase, MD, clarifies a question for Ray Renken, graduate student in the UIUC Department of Physics. (Credit: Jack Gladin, CSL)

Simultaneous with SIGGRAPH '89 in Boston was the Massively Parallel Computing Summer Workshop at NCSA's Computing Applications Building. Two representatives from Thinking Machines Corp., Bernie Murray and Jacek Myczkowski, trained researchers together with NCSA staff in the use of a massively parallel computer such as the Connection Machine model CM-2. At this writing, NCSA's CM-2 has been installed in the Beckman Institute and is undergoing a friendly user period [see opposite page]. Dedicated Connection Machine time for the workshop's hands-on activities was provided by Thinking Machines Corp., Cambridge, MA. Further information about the workshop is available from Michael Welge, acting associate director of the Applications Group, who coordinated and planned the event [see **NCSA Contacts**, page 19].

NCSA's Connection Machine (Model CM-2) newly installed at the Beckman Institute. Although the technology for producing each customized chip (at 16 processors per chip) is similar to that used in personal computers, the machine's speed is attributed to the power of its 32,768 processors working together to solve a problem.

Connection Machine installed

by Jarrett S. Cohen, Public Information Specialist

NCSA recently installed its newest supercomputer, a Thinking Machines Corp. Connection Machine Model 2 (CM-2). The machine is housed at the Beckman Institute for Advanced Science and Technology.

The CM-2 is one of a new breed of computers known as massively parallel, which contain large numbers of processors. Whereas conventional supercomputers contain from 1 to 8 general-purpose scientific processors, the CM-2 can be configured with as many as 65,536 data parallel processors (NCSA's model has 32,768). This architecture makes the CM-2 especially suitable for scientific problems in which the same computational operation is applied to large numbers of data items.

NCSA will run the CM-2 in tandem with its CRAY X-MP and CRAY-2 systems to expand the computational capabilities provided to academic and industrial users across the U.S.

The $3.16 million machine was provided to NCSA by the Defense Advanced Research Projects Agency (DARPA) in cooperation with NSF. The Connection Machine architecture was developed by Thinking Machines Corporation under DARPA's Strategic Computing program.

"I am very excited that NCSA will be able to provide national access to the Connection Machine," said Director Larry L. Smarr. "The Connection Machine is one of the first massively parallel supercomputers. I think it will open many new areas of applications, because certain important problems will be much better adapted to its architecture rather than the more familiar architectures of current supercomputers."

The CM-2 is well suited to mapping certain natural phenomena, as its large number of processors can be programmed to imitate their behavior. It has been used for a wide variety of applications, including artificial intelligence, visualization, and weather modeling.

As the CM-2 is a relatively new architecture, the NCSA Parallel Processing Program has defined "Grand Challenge" projects that will be "sought out for their potential in generating new algorithms and software useful to the broader user community," said Michael Welge, associate director for Applications.

Grand Challenge areas include computational fluid dynamics, general relativity, medical imaging, engineering mechanics and design synthesis, genome analysis, Monte Carlo simulation, lattice gauge theory, molecular modeling, condensed matter, and electron devices, Welge said.

A friendly user period lasting through December has been established to integrate the CM-2 into NCSA's computational environment.

Proposals for time will be reviewed by the joint NCSA/Pittsburgh Supercomputing Center Peer Review Board quarterly beginning in December. Proposals are due by November 1 for the December meeting. Proposals for fewer than 100 hours are reviewed by the Small Allocations Committee, which meets monthly.

For further information, contact Michael Welge (see **NCSA Contacts**, page 19). ▲

Training dates, 1989

Oct. 9–12	New User Training
Oct. 23–24	**User Group Meeting** (see page 11)
Nov. 6–10	Affiliates Training
Dec. 11–14	New User Training

Note: Dates are subject to change. You must register to attend NCSA training. Class size is limited.

To register: Academic users contact Kendra Reasor at (217) 244-1100. Industrial partner users contact your representative at NCSA.

Additional information: contact Janice Knapp-Cordes at (217) 333-0085 or at janicek @ncsa.uiuc.edu (Internet).

Winkler continued from page 9

Students are the main output of universities, and Winkler is looking forward to working with students at all levels. Many degrees of specialized knowledge, concepts of theoretical experimentalists as well as machinery and logistics problems of laboratory experimentalists, and varying skills of people must all come together to perform numerical simulations.

Pioneer computational scientist

A native of West Germany, Winkler studied physics at the University of Göttingen and worked for nine years at the Max Planck Institute for Astrophysics near Munich. His long-time collaboration with Larry Smarr (NCSA director) and Michael Norman (NCSA research scientist) began nearly a decade ago—twice as long as the NSF supercomputer centers program has existed—when he invited them to Germany where they modeled extragalactic jets on the supercomputer at Max Planck [see ***access***, May–June 1989]. Winkler's current scientific interest is time-dependent multidimensional continuum physics.

In this country Winkler has been associated with the Los Alamos National Laboratory, the Lawrence Livermore National Laboratory, and the University of California at Berkeley. He has served on several advisory committees to the National Science Foundation and the National Institutes of Health. For approximately two years he sat on the NCSA/PSC Peer Review Board. Recently he accepted an invitation to be a visiting scientist at the Numerical Aerodynamics Simulator Project, NASA Ames Laboratory.

Since his immigration to the United States about five years ago, Winkler says he has "concentrated on conceptualizing and establishing a constantly evolving, well-balanced computational environment for scientific and engineering purposes." ▲

ABC airs NCSA visualization

by Dan Brady, Manager, Visualization and Media Services

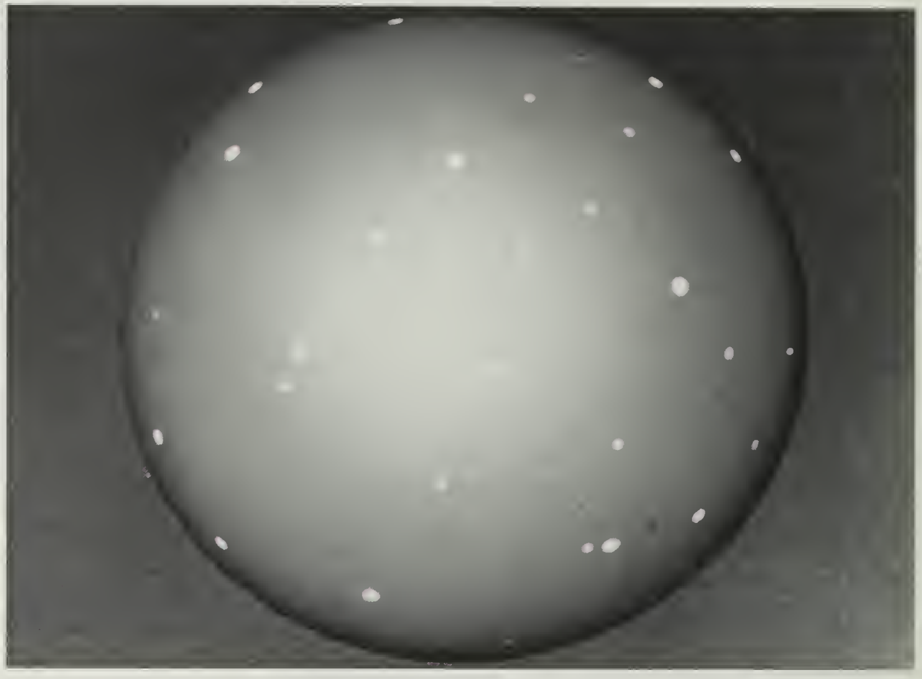


Image from NCSA's visualization shown on ABC-TV.

The Visualization Group produced a visualization illustrating the "big bang" and "final crunch" (beginning and end) of the universe for "20/20," the ABC network TV program. NCSA's visualization was used for a biographical segment on the renowned British physicist Stephen Hawking.

The segment was shown Friday, July 7. The expanding "balloon-like" image used during Hugh Downs' interview with Hawking was from NCSA. At the end of the program, credit was given to NCSA.

This visualization was produced by Jeffery Yost and Mark Bajuk, scientific animators. Larry Smarr, NCSA directore, and David Hobill, postdoctoral research associate, provided consulting expertise on the physics of the event.

With this visualization, NCSA's Visualization Group made its commercial network TV premiere. ▲

Donations to NCSA

NCSA thanks John L. Larson, NCSA senior research scientist [see ***access***, November–December 1988], for his generous donations to NCSA.

For several years he has made a contribution to NCSA. An alumnus of UIUC, he earned a Ph.D. in Computer Science in 1978.

This year's gift has been earmarked for the library or for training. NCSA appreciates these types of donations since they allow freedom in their use.

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General information and machine access

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FAX (217) 244-1987

Orders for Documentation and Publications
Kay Weidner
(217) 244-8045

Cray Operations
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Dialup Access—2400 baud or less
(217) 244-0662

Dialup Access—9600 baud
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CRAY X-MP IP address
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Online Notes

Updated online information

by Will Ridenour, Online Documentation Editor

The following online documentation has been added or updated as of September 9, 1989:

UNICOS man pages

Name	Description
abaqus	Finite Element Analysis Program
acm-alg	Collected algorithms of the ACM
bmin	Macromodel batch minimizer
cfs	Accesses the Common File System
cftmath	General purpose math library
chemistry	Describes chemistry applications
compress	Compresses datafiles
ds	Reports free disk space on file systems
help	Accesses the hierarchical help system
kermit	Transfers files between mainframes and microcomputers
merge	Three-way file merge
nprint	Prints files on UIUC printers
space	Reports free disk space on scratch and home file systems
zoom	Zero/one optimization program

To view a man page, enter: **`man`** ***`manpage`***
where *manpage* is the name of the man page you wish to read.

UNICOS help files

Topic Name	Description
catalog	NCSA *Technical Resources Catalog*
fortran	Information on the Fortran programming language
finding-information	Finding information online
security	Security issues and information
software	Latest information on applications available on NCSA machines
training	Information on training available to NCSA users
unicos	Information on using UNICOS systems at NCSA
unicos5	Information on the coming upgrade to UNICOS 5.0

To view a help file, enter: **`help`** ***`topic`***
where *topic* is the area about which you want information.

UNICOS documents

Topic Name	Description
datalink	Full text of all 1989 ***data link*** issues
kermit.doc	Documentation for the kermit file transfer protocol
kermit.update	Updates on the kermit file transfer protocol
online.list	Complete list of all online information available at NCSA
users-guide	NCSA *User's Guide*
zoom	Documentation for the zoom zero/one optimization program

To view a document, change your working directory to /usr/local/doc and enter: **`more`** ***`docname`***
where *docname* is the name of the document you wish to view.

data link Contents

- Notes and quick tips
- Hot topics in the NCSA Consulting Office
- Improving your odds with NQS jobs
- Estimating memory requirements for executable files on the NCSA Cray systems
- A cdbx tutorial
- ITPACK available on the CRAY X-MP/48 system
  LAPACK available on the NCSA Cray systems
- PCGPAK updated on the CRAY X-MP/48 system

If you want to receive a copy of the current ***data link***, contact the NCSA receptionist at (217) 244-0072.

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152 Computing Applications Building, 605 E. Springfield Ave., Champaign, IL 61820.

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Software

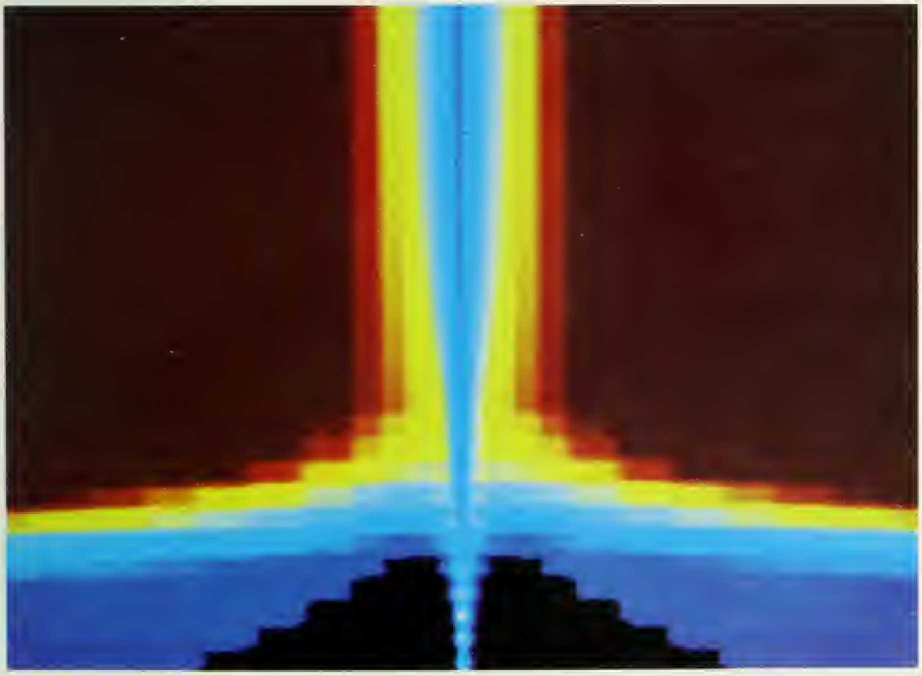
Modeling the San Andreas Fault with NCSA software

by Jill Peacock, Editorial Assistant, Software Tools Development Group

Research on the San Andreas Fault by Dr. Gregory Lyzenga of Jet Propulsion Laboratory (JPL), Pasadena, CA, and Dr. Arthur Raefsky of Stanford University, Stanford, CA, was one of the many scientific efforts included on the recently released Apple '89 compact disc (CD) shown at SIGGRAPH '89 [see ***access***, July-August 1989].

By manipulating their data using the NCSA Scientific Visualization Software Suite—also included on the CD—these scientists were able to generate images from their data to create a better understanding of their study and the models used in it. "Since we've started using NCSA's visualization tools, there's been a substantial change in the way we've interpreted and modified our models. The basic techniques we've been using to model stress on the faults haven't changed a great deal over the last three or four years, but the manner in which we've interpreted those models, modified them, and looked at them has been radically changed by the introduction of the visualization tools," says Lyzenga, technical group leader in charge of crustal deformation modeling in the Space Geodetic Science and Applications Group.

Simulation of the migration of stress through the Earth 6 years after an earthquake (Courtesy NCSA/STDG and authors).



Advancing scientific understanding

Lyzenga and Raefsky study the mutual relationships between earthquakes and stress on faults via numerical models. In doing so, they take particular account of plate tectonic motion occurring in the San Andreas Fault region. "At the boundary between the Pacific Plate and the North American Plate, the motion is predominantly what we call 'strike-slip.' It's a lateral motion. So the motion on the San Andreas Fault is horizontal with Los Angeles moving toward the northwest and San Francisco moving relatively to the southeast," explains Lyzenga.

***Fault** continued on page 3*

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Dear Readers:

With the next issue of ***access***, the newsletter will be published monthly. NCSA is continuing to grow in its service to the research community, and this growth is reflected in the need for additional coverage of center activities.

Sincerely yours,
Fran Bond and Stephanie Drake, editors

*Note: Italicized titles indicate boxed information. Since boxes are fillers, their subjects may not follow the topics of the heads under which they fall.

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Abbreviations

CRI	Cray Research Inc.
CSRD	Center for Supercomputing Research and Development
IRC	Interdisciplinary Research Center of NCSA
NCSA	National Center for Supercomputing Applications
NSF	National Science Foundation
UIC	University of Illinois at Chicago
UIUC	University of Illinois at Urbana-Champaign

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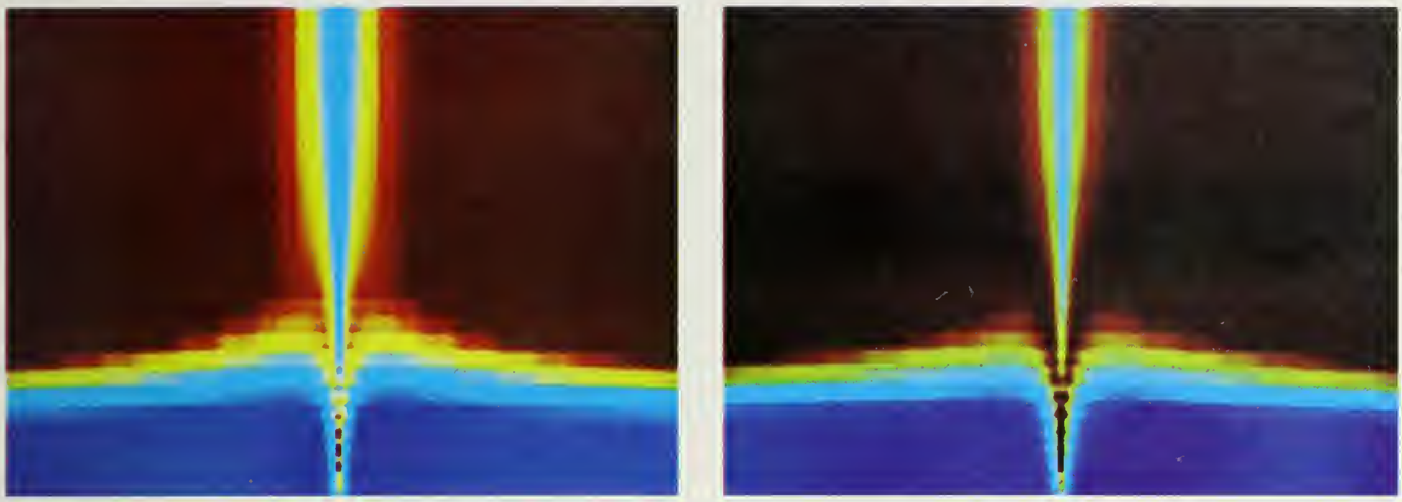
***Fault** continued from page 1*



Simulation showing the migration of stress through the Earth at 76 years after (left) and 156 years after (right) an earthquake (Courtesy NCSA/STDG and authors).

Lyzenga describes the main focus of their work as follows: "We have a certain amount of historical information on the location and timing of earthquakes on the San Andreas Fault, but it's limited. We also have a limited understanding of the sort of microscopic-physical processes that determine how rocks deform and how they break. But there's a gap in connecting these two realms—things that happen on the laboratory scale, and things that happen in the Earth. The purpose of our modeling is to try to bridge that gap and gain a better understanding of what happens on time scales of months to years and to understand better just exactly how the Earth works as a system.

"It's certainly an overstatement to say we're working toward earthquake prediction, because at this point we really don't know all the elements that go into governing every single earthquake. It may be that earthquake prediction is one of those things that in principle is impossible—like weather prediction is in principle almost impossible beyond a certain length of time. What we're doing here is trying to explore the basic physics and find out what the important governing properties are in determining when and how earthquakes repeat on a fault zone. We are examining the influence caused by assuming different material properties, different driving rates, and different geometries on the fault and comparing the results with what limited data we have from the field and from the laboratories."

Exposing errors

To generate their research models and compare the influence of different assumptions, Lyzenga says he and Raefsky used a "finite element method to generate a large list of displacements and stresses characteristic of each model. Before having the visualization tools, we had to look at big tabulations of numbers and try to figure out what was going on."

Because the appropriate software wasn't available in the earlier stages of their research, the scientists could only resort to creating contour plots and taking one-dimensional slices through their data. Lyzenga explains the limitations of this process and how the NCSA software helped out. "It took a lot of time to try many different scenarios and tweak parameters to see how they looked under different conditions. ...As soon as we had the visualization tools, it immediately became much easier to see where we were having problems with our technique. We sometimes had numerical oscillations or other shortcomings in the computational technique.

"The other aspect of it was extracting the scientific content. Once we had the thing working correctly, it was straightforward to separate interesting phenomena from spurious effects. Being able to get in there and play with the palette and enhance the solution in some particular area or another has really helped a lot in our ability to extract meaningful information.

"The interesting example from our recent work involved the process of moving our finite element code between different platforms. We've been doing work on various minicomputers, parallel processing hypercubes, and also on Crays. Usually if you make a big mistake, everything will just crash and burn, and it's obvious there's something wrong with the program. But at the same time, we're trying to explore some fairly unusual behaviors in the way faults fail and accumulate stress. It's not always clear whether the answer you're getting out is right or not.

"A couple of months ago I thought I had wrapped up a working version of the finite element code for use on some production results. We let it crank up and run overnight. We got some answers which seemed a little bit unusual, but not all that far out of the ballpark.

"Previous to having NCSA Image, I probably would have examined the output file by looking at a few numbers by hand and concluding, 'Oh, that looks like it worked.' Instead, what I'm able to do now is quickly run the output through a filtering program that puts it into HDF format [Hierarchical Data Format] and zoom it up on DataScope or Image. Doing so, it was instantly apparent from a look at the screen that there was a serious numerical oscillation in the solution. Without the help of these visualization

***Fault** continued on page 22*

Cooking with Crays: parallel processing

by Kathleen Robinson, Science Writer

John Larson.

Just over a year ago, Dr. John Larson joined the staff at NCSA as a research scientist to continue work on the performance evaluation of parallel and individual processors he began as a senior applications engineer at Cray Research Inc. (CRI) [see ***access***, November–December 1988]. His other research interests include user education, algorithm design, and language development for parallel processing.

User training in multiprocessing is a significant part of Larson's work at NCSA. As one accustomed to explaining the issues of parallel processing to audiences, he has an analogy ready. "I like to compare parallel processing on computers with the task of getting dinner ready on time. The trick is not only to identify those things you want to prepare for dinner and get all the burners on your parallel processing stove working simultaneously, but also to have everything ready to eat at the same time. These concerns are very basic in writing programs for parallel machines—you want to keep the burners busy and you want everything to finish together. I sometimes worry about job security," he jokes, "with so many cooks experienced in parallel processing."

Performance workbench project

Larson's principal project now is the development of a performance workbench for the Cray environment to help researchers determine whether their code is working optimally. Analysis tools contained in the workbench will include graphic displays to help users visualize bottlenecks to the performance of their code. The workbench project was recently approved for funding by NSF. Larson and Dr. Kyle Gallivan and Allen Malony of the Center for Supercomputer Research and Development (CSRD) are the principal investigators.

Larson explains, "The tools in the performance workbench will collect information at different levels from a program either before it executes or as

Scientific visitors

Andrew Abrahams
Affiliation: Cornell University
Date: October 7–13, 1989
Area: *Astrophysics*

Bernhard Bernu
University of Paris
October 25–November 3, 1989
Chemistry

Ken Bishop
University of Kansas
October 16–17, 1989
Petroleum Engineering

Tom Bouman
Southern Illinois
University–Edwardsville
August 30, 1989–August 15, 1990
Quantum Chemistry

Michel Caffarel
University of Paris
November 6, 1989–October 30, 1990
Chemistry

Aage Hansen
Oersted Institute
Copenhagen, Denmark
October 6–27, 1989
Quantum Chemistry

John Hawley
University of Virginia
September 28–October 3, 1989
Astrophysics

Helga M. Leonhardt Hendriks
Leonhardt Language System, Inc.
October 21–26, 1989
Linguistics

Daniel Puckett
University of
Arkansas–Fayetteville
October 25–26, 1989
Graphics

Philip Stevens
University of Southern California
October 19–22, 1989
Physical Chemistry

it executes, then filter the results to graphics utilities that the user can interact with." One proposed tool is being developed by Malony and UIUC graduate student David Bradley. This tool will enable researchers to see which component of the machine is limiting performance through the use of a display similar to those used for tracking critical resources in manufacturing projects. For example, the display may show that the factor limiting performance is the rate at which data moves back and forth to memory. Using this tool, a researcher will be able to see where optimization efforts would be best spent.

Another aspect of the workbench project is for Larson and Gallivan to do parallel and vector algorithm development to search for more questions that need answering. Situations that arise as they explore algorithm-hardware interactions will suggest additional performance analysis tools that should be developed.

Work with NCCE

Larson has a joint appointment with the National Center for Computational Electronics (NCCE), recently formed at UIUC with Dr. Karl Hess as director [see ***access***, September–October 1988]. Larson first worked with Hess several years ago at CRI to collaborate on an early visualization of electron flow. Laughs Larson, "It was a visualization which by today's standards would look like balls and sticks. But four years ago when no one else was presenting things visually, it was quite something." Larson also vectorized and parallelized the code Hess was using as a demonstration of the applicability of parallel processing to the area of device simulation. The optimized code ran 563 times faster on the CRAY X-MP supercomputer than on Hess' departmental machine (at that time, a Harris 800 48-bit superminicomputer).

Larson is now working with NCCE graduate student Vadim Pevzner on a program that involves following the path of individual electrons through a transistor. "Imagine light coming through windows into a room," Larson says, "then reflecting off several irregular surfaces inside the room. In our program, the light represents electrons. They bounce off the walls and eventually either go back out where they entered (they are reflected), or they exit another window as output (they are transmitted). Whether the electrons are reflected or transmitted is a basic property of how the transistor works.

"Because each of the electrons goes through the device independently, each of them can be tracked by a different processor. The multiprocessing aspect of the code is easy. The difficult part is how to do the parallel processing and make use of the vector capabilities of the CRAY-2. To do that, we have to organize the computation so we can work with many particles at the same time and operate on the information associated with those particles uniformly. We're trying to get the benefits of both capabilities of the machine—parallel processing and vectorization—in order to get the fastest program and to do the most analysis."

> *"I like to compare parallel processing on computers with the task of getting dinner ready on time. The trick is not only to identify those things you want to prepare for dinner and get all the burners on your parallel processing stove working simultaneously, but also to have everything ready to eat at the same time."*

Hardware performance monitor

The CRAY X-MP and Y-MP lines of computers have a useful hardware performance monitor that automatically collects performance information about every program that is run. While he was working at CRI, Larson wrote some software that makes the hardware performance monitor more useful by allowing researchers to obtain performance information without modifying their code. "It's all in the way they submit their program," he says.

Larson advocates utilizing the hardware performance monitor because researchers who use it almost always go on to develop more effective code. "Getting a low performance number is a bit embarrassing at first," he says, "and you don't want to tell everyone that your program is running slowly. With performance information, the user can benefit and NCSA as a whole can benefit. The user can better understand the efficiency of a code (and perhaps how to improve it) and can make a better case to the resource allocation board, showing the code's suitability in a supercomputer environment. The site can better understand system utilization for the purpose of offering help to inefficient users and for capacity planning."

Matching hardware and software

"One thing that's different about this kind of science," says Larson, "is that it's not like physics or chemistry where there are laws of Nature. We study specific interactions between hardware and software. The interactions are governed by the rules of the particular hardware which (unfortunately) are not publicized by the vendor. When a machine comes out with new capabilities or you're looking at a collection of different machines, then how you write your program—and how to make best use of that architecture—is different.

"We're at a point where parallel computing will become the default mode, rather than sequential computing," predicts Larson. "We'll be doing many things at the same time and have an organization of computers or processors at work, rather than just one. This requires some rethinking about how to write programs and how to build machines that can execute those programs effectively.

"Just looking at peak performance is not a good measure of a machine. Peak performance doesn't necessarily—and usually doesn't—indicate how well the machine will perform on your program. The important thing is finding the right tools to solve your problem—the right hardware, the right software—and, critically, harmony between them." ▲

Allocation meetings

by Patricia Wenzel, Manager, User Administration

NCSA has been listing allocations approved by the Peer Review Board (PRB) for some time. This report also includes allocations approved by the Small Allocation Committee (SAC).

We welcome proposals from the national research community.

The PRB recently made a change in policy that affects which committee acts on a proposal. In the past, the PRB has reviewed any proposal where the lifetime total allocation requested was 100 or more service units (SUs). In the future, the PRB will review only those proposals where the SUs in a given year equals 100 or more. (The SAC will review those under 100 SUs.) Multiyear requests are encouraged. The PRB requires review of a progress report at the end of each year.

Joint NCSA/PSC Peer Review Board Meeting—September 28, 1989

Principal investigators and their approved projects are as follows:

S. I. Abdel-Khalik, Georgia Institute of Technology, *SRP Confinement System Modelling*, CRAY X-MP/48, 10 SUs.

James B. Adams, University of Illinois at Urbana-Champaign, *Theory and Computer Simulation of Metallic Interfaces*, CRAY X-MP/48 and CRAY-2, 100 SUs.

Bruce Allen, Tufts University, *Inflationary Cosmology, Cosmic String Models and the Vilkovisky-DeWitt Formalism*, CRAY-2, 30 SUs.

David Arnett, University of Arizona, *Supernova Hydrodynamics*, CRAY X-MP/48, 1000 SUs.

Michael W. Berry, University of Illinois at Urbana-Champaign, *Row Projection, Neural Network, Banded Linear System, and Singular Value Decomposition Algorithm*, CRAY X-MP/48 and CRAY-2, 350 SUs.

R. Stephen Berry, *University of Chicago, Few Body Dynamics in Atoms, Molecules, and Clusters*, CRAY X-MP/48 and CRAY-2, 150 SUs.

David A. Brant, University of California–Irvine, *Conformational Dynamics of Oligosaccharides*, CRAY-2, 150 SUs.

David F. Coker, Boston University, *Development of Simulation Methods to Study Nonadiabatic Nuclear Dynamics of Solvated Electron Systems*, CRAY-2, 400 SUs.

Subhendu Datta, University of Colorado, *Wave Propagation and Scattering in Composite and Heterogenous Media*, CRAY X-MP/48 and CRAY-2, 50 SUs.

Ernest Davidson, Indiana University, *Molecular Interactions*, CRAY-2, 300 SUs.

Arthur Freeman, Northwestern University, *Electronic Structure of Bulk Solids and Surfaces and Electronic Structure of Artificial Materials*, CRAY X-MP/48 and CRAY-2, 3000 SUs.

Peyman Givi, S.U.N.Y. at Buffalo, *Direct Numerical Simulations and Large Eddy Simulations of Unpremixed Turbulent Reacting Flows*, CRAY X-MP/48, 75 SUs.

Christoph K. Goertz, University of Iowa, *Investigation of Microscopic and Macroscopic Plasma Properties*, CRAY X-MP/48, 185 SUs.

Michael Grossman, University of Illinois at Urbana-Champaign, *Estimation of Genetic Parameters for Somatic Cell Count in Milk*, CRAY-2, 20 SUs.

A. D. J. Haymet, University of Utah, *Molecular Level Theory for the Action of Fish "Antifreeze" Glycoproteins (AFGPs) and Polypeptides (AFPs)*, CRAY X/MP 48, 200 SUs.

Warren J. Hehre, University of California–Irvine, *Development and Parameterization of Intermolecular Potentials for Molecular Dynamics and Monte Carlo Simulations*, CRAY-2, 250 SUs.

Paul E. Kilbride, University of Illinois at Chicago, *Quantitative Ophthalmology of Ocular Pigments*, CRAY-2, 50 SUs.

John Kogut, University of Illinois at Urbana-Champaign, *Optimizing Algorithms for the Cray-2 and Cray-3*, CRAY-2, 1000 SUs.

Randy L. Kolar, University of Notre Dame, *Numerical Simulation of Surface and Subsurface Flow Phenomenon*, CRAY X-MP/48, 50 SUs.

Kin Lam, University of California–Goleta, *Numerical Simulation of Turbulent Flow with a Free Surface*, CRAY X-MP/48, 100 SUs.

Paul C. Lauterbur, University of Illinois at Urbana-Champaign, *Computational Support for Investigation Using 3D NMR Microscopy*, CRAY-2, 400 SUs.

Allan MacDonald, Indiana University, *Strongly Correlated Quantum Systems*, CRAY X-MP/48, 200 SUs.

Richard Martin, University of Illinois at Urbana-Champaign, *Electronic Structure of Condensed Matter*, CRAY-2, 550 SUs.

Richard Matzner, University of Texas–Austin, *Problems in Gravitation*, CRAY-2, 100 SUs.

James J. Riley, University of Washington, *Supersonic Shear-Layer Flow*, CRAY X-MP/48 and CRAY-2, 100 SUs.

***Allocations** continued on page 21*

Tom Bouman—visiting chemistry professor at NCSA

by Joe Golab, Applications Scientist, Computational Chemistry Group

Thomas Bouman (left) and Aage Hansen (right).

Dr. Thomas Bouman is spending a sabbatical year with NCSA as a visiting professor in the Computational Chemistry Group. Bouman, whose expertise is in quantum mechanics, is a professor of chemistry at Southern Illinois University at Edwardsville.

Two years ago he served as the National Science Foundation program officer in the Quantum Chemistry Program. In that capacity, he was responsible for the grants program in quantum chemistry and made recommendations for funding proposals.

In his "spare" time, Bouman also codevelops and maintains the robust program for Random Phase Approximation Calculations (RPAC) with Dr. Aage Hansen, a chemistry faculty member at the Oersted Institute in Copenhagen, Denmark. During October, Hansen visited NCSA to work with Bouman.

Manipulating RPAC

Since his arrival at NCSA in August, Bouman has focused his energies on optimizing and enhancing the performance of RPAC (QCPE #556) on NCSA's Cray systems. RPAC is an integrated suite of codes that uses the output from a standard self-consistent field (SCF) program—such as GAUSSIAN86, HONDO 7.0, or GAMESS—and performs post-SCF computations. The package can calculate electronic excitation energies, oscillator and rotatory strengths, transition densities and excitation charge rearrangements, and nuclear magnetic resonance (NMR) shielding tensors. In addition, it provides analyses in molecular structural terms and graphic output for these quantities.

RPAC is already used at laboratories around the world—academic and industrial. Right now, RPAC can handle all the particle-hole configurations generated by up to 255 atomic basis functions. Because of the capabilities that RPAC allows for post-SCF calculations, it will be a welcome addition to the NCSA computational chemistry library of applications software [see ***datalink***, July–August 1989].

Bouman plans to leave a public copy of the RPAC executable on both Cray systems. Persons interested in the source code should contact him directly.

Utilizing the Crays

"I decided to come to NCSA because of its unique combination of supercomputer resources and its emphasis on scientific visualization," says Bouman. "For example, I am making use of the large memory on the CRAY-2 supercomputer to develop an in-core formulation of second-order linear response methods for calculating molecular properties. The only other implementation we know of is heavily I/O bound and thus limited to relatively small systems."

Bouman is also extending his localized orbital methods to compute vibrational circular dichroism and is investigating the use of effective core potentials in the determination of heavy-atom NMR chemical shifts. While at NCSA, he will hone his vectorization skills on the Cray machines and work on better methods for graphical output of molecular wavefunctions.

If you would like to contact Bouman while he is at NCSA, his electronic mail addresses are tbouman@ncsa.uiuc.edu (Internet) and 12308@ncsavms (BITNET). ▲

Training dates: 1989-90

1989		**1990**	
Nov. 13–17	New User Training	Jan. 22–26	New User Training
Dec. 11–14	New User Training	Feb. 12–16	New User Training

Note: Dates are subject to change. You must register to attend NCSA training. Class size is limited.
To register: Academic users contact Kendra Reasor at (217) 244-1100. Industrial partner users contact your representative at NCSA.
For additional information: Contact Janice Knapp-Cordes at (217) 333-0085 or at janicek@ncsa.uiuc.edu (Internet)/13036@ncsavms (BITNET).

Linking social science models

by Will Ridenour
Online Documentation Editor

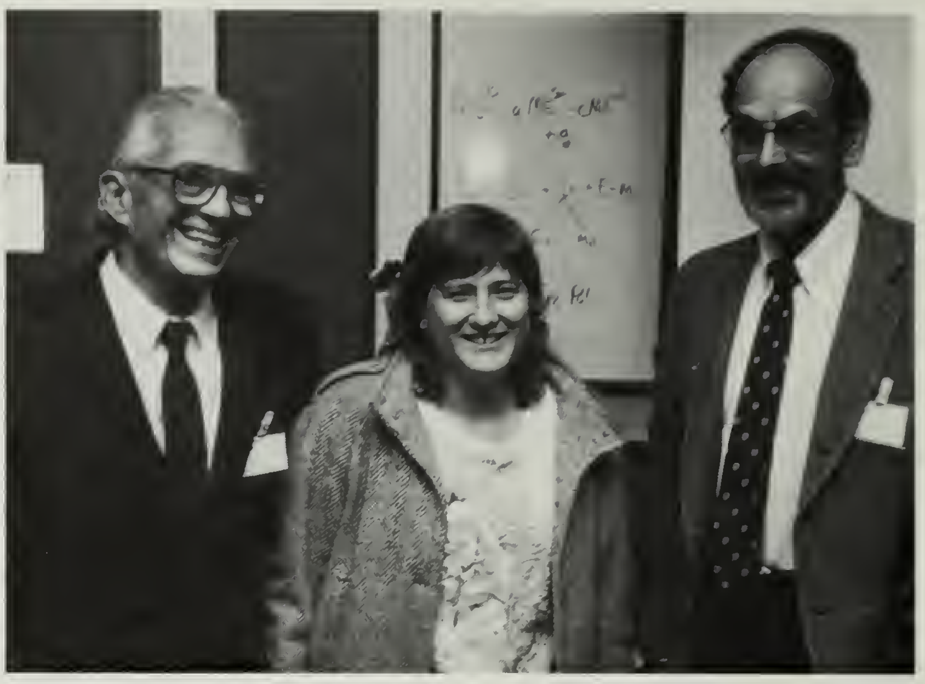
With an eye on helping to provide an effective decision support tool for the problems of pollution and global warming, a group of 22 invited social science modelers spent three days in September at NCSA exploring an integration of their efforts and considering ways that supercomputing might open new possibilities in their field.

Like modelers in the natural sciences, social science modelers build systems of postulates, data, and inferences aimed at a mathematical description of something in the real world. While natural science models describe things like the behavior of an earthquake or a black hole, social science models are representations of mass human behavior in such areas as world trade or the interplay of hostility and cooperation among nations.

The workshop, "Large-Scale Social Science Models on Supercomputers," held from September 26 through 28 at the Beckman Institute, was jointly sponsored by the National Center for Supercomputing Applications and the Cornell National Supercomputer Facility.

Planning for the workshop began several years ago when NCSA's Dan Alpert, associate director for Faculty Programs, heard Dr. Walter Isard, professor of economics at Cornell University, speak on the UIUC campus about peace science. Isard is a member of the Peace Science Society, a group of interdisciplinary scholars concerned with analyzing conflict and using the tools of science to find peaceful solutions to global problems. When Alpert told NCSA Director Larry Smarr about Isard and his work, the seeds for the workshop were planted.

> *"We wanted to find ways to pull together all the different economic, trade, and social models into a global model that could be used for decision support and eventually, for input into the global climate and ecological models."*



Left to Right: Walter Isard, Christine Smith, and Sidney Saltzman.

"This was part of our attempt to bring together people in the subfields of the social sciences and natural sciences to see if there are emerging disciplines," said Smarr.

Analyzing interactions

According to workshop participant Richard Schuler, professor of economics at Cornell and director of Cornell's Waste Management Institute, peace science can be viewed as an attempt to analyze interactions among social science systems. "Breakdowns in the sociopolitical system are affected by and forge change on the economic and demographic systems," he explained.

Finding ways to reflect this fundamental interconnectedness in their models was the workshop attendees' goal. "We got together to review the field and to see if we could couple models together," said Isard. "We wanted to find ways to pull together all the different economic, trade, and social models into a global model that could be used for decision support and eventually, for input into the global climate and ecological models."

Making connections

Each session had a general theme leading toward those goals. The first morning looked at "The Operational Integration of Models" with papers by Sidney Saltzman, professor of city and regional planning at Cornell; Christine Smith of the School of Administration, Griffith University, Australia; Dr. Isard; and Jeffrey Bergstrand of the Department of Finance, College of Business Administration, University of Notre Dame.

The second session focused on the LINK world econometric model, developed by Nobel laureate Lawrence Klein and his associates at the University of Pennsylvania, with a paper by Christian Petersen of The World Bank and another on using the LINK model to model the impacts of military expenditures by Klein and Miroslaw Gronicki of the Department of Economics at Pennsylvania. NCSA Director Larry Smarr capped the first day with an overview of trends in supercomputing and their potential benefits for the field of social science modeling.

The second morning's session explored two of the major types of economic models with papers by Faye Duchin of the Institute for Economic Analysis, New York University, and Eric Thorbecke, professor of economics at Cornell. Richard Schuler, also of Cornell's Department of Economics, finished the second morning session with an look at issues involved in integrating global and regional models.

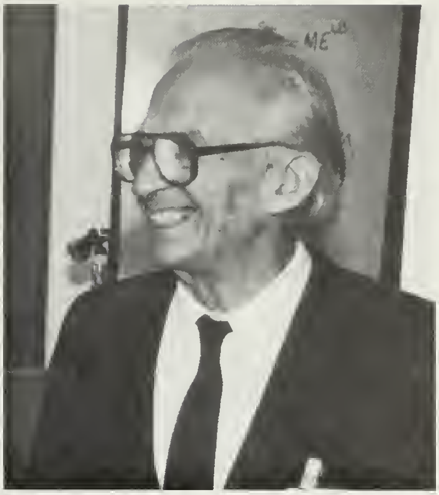
The afternoon sessions looked at some alternative models with papers on the GLOBUS world computer simulation by Stuart Bremer, professor of political science at SUNY–Binghamton and Barry Hughes of the Graduate School of International Studies, University of Denver; and a paper by Steven Seitz, Dina Zinnes, and Robert Muncaster, of the Merriam Laboratory for Analytic Political Research at UIUC.

The final day of the workshop focused on "Linked Subnational Models" with papers by Sidney Saltzman; Tim Mount of the Department of Agricultural Economics at Cornell; and Geoffrey Hewings, professor of geography at UIUC. Afternoon sessions consisted of summaries by Isard, Smith, and Saltzman—first for the workshop and then, in the Beckman Auditorium, for the campus community.

The World Bank and environmental impact

Just as the workshop got underway, an announcement from The World Bank underscored the importance of the workshop's goals. According to an Associated Press story, World Bank President Barber Conable had told delegates to the annual meeting of The World Bank and the International Monetary Fund that his agency is building environmental impact assessments into its loan review and that they were reviewing "such issues as the Third World debts crisis, the political upheaval in Eastern Europe, and the efforts needed to keep huge trade imbalances from derailing the global economic expansion."

The World Bank's new position follows world trends as national and international organizations begin to consider the environment as at least as important as the economy and to understand that environmental problems are strongly coupled to economic activity. In aiming for the increased comprehensiveness of linked social science models, the workshop participants were taking the first steps toward providing an effective way for national and international policymakers to consider all the consequences of their decisions.



Walter Isard.

The mathematics of noise

A workshop paper by Tim Mount, professor of resource economics at Cornell, and Martha Czerwinski, systems analyst with Cornell's Department of Agricultural Economics, provides a key to why linked models are necessary. Dr. Mount reported on a study of the implications for restricting power plant emissions in selected regions of New York State in which simulations showed that heavy reductions in coal use had the most significant effect in cutting emissions of carbon, sulphur dioxide, and nitrogen oxide. Although Mount pointed out that reduced coal use will have many economic, social, and political implications, this was the researchers' conclusion and not something within the scope of the model.

> *"The social scientist feels that the predictive value of the exercise is improved if even an admittedly inaccurate human response is added, compared to ignoring it altogether."*

Isard and his colleagues believe that their more comprehensive, linked models will be able to offer policy makers a clear look at many of the implications of their decisions. The road to making those linkages will not, however, be a smooth one.

Because they deal with the complexity of human behavior, social science models have had to deal with a degree of uncertainty, or what several workshop participants called *noise.* According to Schuler, noise may be a problem in making the eventual connections to global climate and ecological models developed by natural scientists. Physical scientists might be glad to incorporate human responses into their models, Shuler said, "if only the social scientists could get their act together and come up with some reliable 'laws' of human behavior."

Rather than purify their models, however, workshop participants were looking for ways to better deal with uncertainty. "The social scientist feels that the predictive value of the exercise is improved if even an admittedly inaccurate human response is added, compared to ignoring it altogether," said Shuler.

The art of understanding

In order to deal with that uncertainty and with the complexity of their models, social science modelers will need the tools that can be provided by supercomputing such as larger datasets, faster run times, and a tool that may bring a few surprises with it—visualization.

Answering a workshop participant who feared that using visualization in his work would result in a lessening of analytic powers, NCSA Director Larry Smarr replied that to some degree the fear was justified, but that it was a lessening of total reliance on

Interconnections *continued on page 10*

analytic capabilities, while bringing the power of intuition and visual understanding to bear on the problem. "Our education overtrained us in the use of only one side of our brain and mostly ignored the other, the side that artists use," he said. "Of course it feels strange at first, because you're not used to it, but it becomes a very powerful tool for understanding what is going on in our models."

Workshop participants got a first glimpse of the possibilities when they viewed a prototype visualization tool for their field produced by NCSA Industrial Consultant Michael Krogh. Working with Cornell's Bill Dean, Krogh used the Silicon Graphics workstation's graphics library to produce a visual front-end and post-processor for a world economic model. The prototype allowed manipulation with a mouse of such variables as pollution, population, and investment. When all variables were set as desired, the changes went to NCSA's CRAY-2 for processing and then were returned to the workstation for viewing and further manipulations.

"I think the prototype shows how easy it would be to put together useful pre- and post-processors for a model like this," said Krogh. "With additional work between social science modelers and graphics programmers, a much more useful graphics interface could be put together."

The next step

According to Walter Isard, the workshop went a long way toward accomplishing its goals although a great deal of work remains. "I think we scored several important points toward making a global model operational in providing useful data for policy decisions," he said.

"We're certainly far ahead of where we were two years ago. The next step will involve beginning to work with natural scientists to find ways to link the global social science model to global climate and ecology models."

▲

Attendees

Daniel Alpert
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NCSA

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College of Business Administration

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Department of Economics

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Dina A. Zinnes
UIUC
Merriam Laboratory

Visualization explores the depths of visual perception

by Jarrett S. Cohen, Public Information Specialist

The relatively new field of scientific visualization takes millions of numbers spewed out by a supercomputer and applies the principles of art to effectively communicate their meaning. Color theory, in particular, has been applied to heighten the understanding of previously unseen phenomena.

Human beings react to colors and how colors relate to one another. By changing color relationships, people perceive images differently.

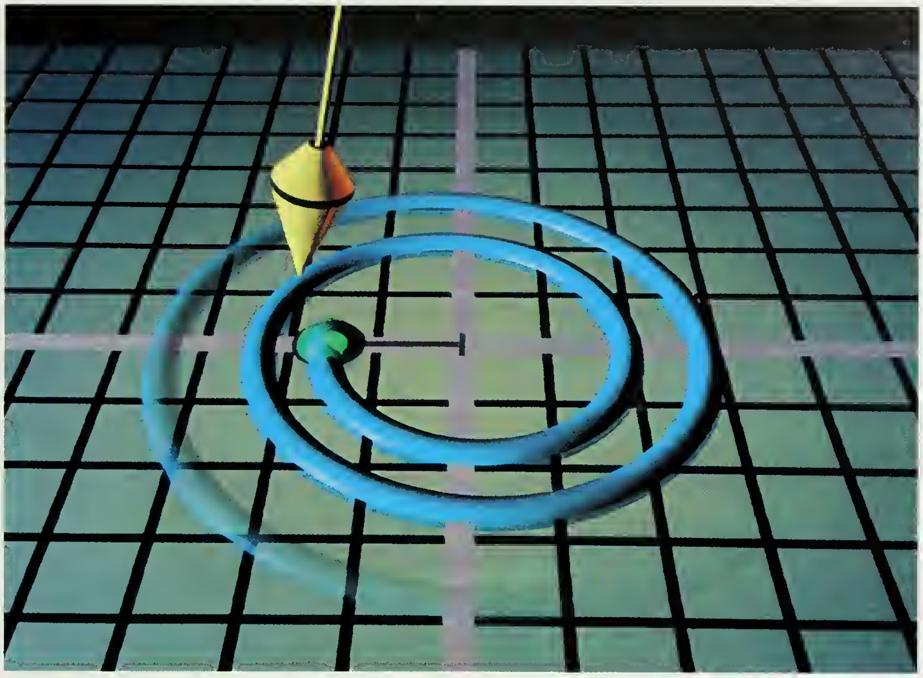
Color, object shapes, and motion are all factors that play a role in human visual perception. To investigate these and other aspects of perception, NCSA's Visualization Development and Services Group (VDSG) recently embarked on two projects that explore how we interact with visual representations—the Data Picture Project and the Human Factors Project.

Data Picture Project

The Data Picture Project takes issues of representation, including color, object form, perspective, and motion sequencing, and investigates their dynamics, according to group manager Dan Brady. "We want to look at the structures of representation—what they are, and how can we use them—in a much broader way than we have in visualization," he says.

Two fundamental structural elements make up the Data Picture Project. Brady describes these elements in terms of a window.

The first is a window opening onto frozen space. He likens this window to a still photo, in which the view is conditioned by the color and the object forms in the space. The second is a window opening onto motion, which "adds the matter of changing the point of view through the window as well as the objects in that window."



Color, object shapes, and motion are factors of human visual perception as this still from an animated visualization illustrates. (Phase diagram of a damped pendulum's movement vs. velocity produced by Mark Bajuk, NCSA scientific animator, and David Hobill, NCSA research scientist and scientific advisor—for a Canadian Broadcasting System presentation on chaos.)

These issues are being addressed in regularly scheduled seminars. Resources include written material and presentations by experts in the fields of photography, cinematography, film theory, and psychology. The group will then take their findings and experiment with them in visualization projects.

"We want to look at the structure first before we impart data on that structure," Brady says. "Many more options will be at hand when we want to put data into the window."

Human Factors Project

"One of the central matters of representation is perception—what is seen by humans through a window of representation," says Brady.

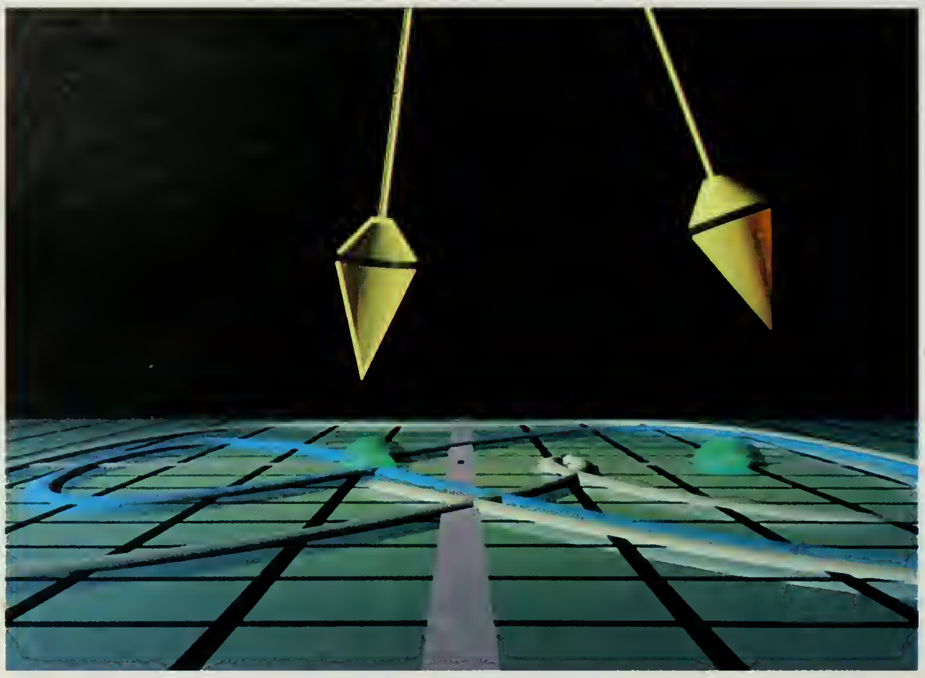
The Human Factors Project is a collaboration with Chris Wickens, head of the UIUC Aviation Research Laboratory and professor in the UIUC Department of Industrial Engineering. It delves into the dynamics of visual perception.

Wickens has done research in this area for the past two years in conjunction with the UIUC Department of Psychology. A human factors psychologist by training, Wickens and his colleagues have investigated "psychological principles of perception of multidimensional data." He cites statistics and air traffic control data as examples of these data.

The basic idea behind human factors research is "applying what we know about perception to the design of displays," Wickens says. Factors that

Perception *continued on page 12*

Still from an NCSA animated visualization illustrating the movement of two chaotic pendulums.



play a role in understanding displays include:

- Color: When is color good? Distracting? How should it be used?
- Three dimensions: How can perspective be used to represent three dimensions of data?
- Motion: What are the dynamics of a display?
- Role of object representation: How can objects be used (e.g., a cube) to represent large amounts of information?

Wickens says these principles are known from fairly basic psychological research. He is now interested in extending them into very complex displays, which include scientific visualization.

A seminar similar to that of the Data Picture Project is the forum for investigation. Other experts have also been invited to share their understanding and expertise.

Collaborative goals

Wickens would like to see experiments in perception and cognition carried out with visualized data. They would provide the VDSG members with "some objective principles for multidimensional display design," he says.

Wickens adds that this collaboration will create a more scientific approach to representation in visualization projects, which he says have "been based more on artistic intuition."

Dan Brady agrees. "By carrying out research in what representation is and how it is perceived, by empirically evaluating these issues, we can find the most dynamic way possible to visualize data," he says. "This is an area that has not been pursued in the field of scientific visualization, but rather in the field of computer–human interaction.

"Linking them—computer–human interaction with scientific visualization ideas—gives us a broader context for developing scientific visualization." ▲

Of music, education, and supercomputing

by Randall Graham, Science Writer

"The common conception is that artists wouldn't have use for a supercomputer and that supercomputer people would think that artists shouldn't be using it," said composer Sever Tipei, UIUC associate professor of music. "Larry Smarr [NCSA's director] had the foresight to attract people in humanities like myself and give them the opportunity to work with the supercomputer."

Tipei is enthusiastic as he speaks about using NCSA's supercomputers in his teaching and his compositions. For Tipei, it's a goal he has pursued for much of his life. Although supercomputers are relatively new, computer music has been around since about 1950. UIUC is one of the places where it originated.

Tipei grew up in communist Romania and studied piano and composition at the Bucharest Conservatory. Writing and performing Western modern music was not allowed there. "Naturally, I knew a lot about contemporary music," said Tipei. "It's the forbidden fruit. I had an interest in computer music even in Romania, although I didn't have access to a computer. And I actually started writing my first computer music program before I ever touched a computer."

Eventually Tipei defected to the West while performing in Holland. Later he completed a doctorate in composition and came to teach at UIUC in 1978. All along he has had a passion for writing computer music, but it was a grant on the supercomputer that finally provided him with the speed and memory his music requires—for Tipei's music is more than notes put on paper with the aid of a desktop workstation.

Beyond Newton

Tipei likes to compare his music to science. As a composer, his purpose,

Left to Right: Robin Bargar, student; Sever Tipei, music professor; and Ben Cox, student.

like that of most scientists, is to help explain the universe and man's place in it. To him, each composition is an experiment—one that requires modern tools and a modern understanding to be a success. At the heart of Tipei's music is the concept of controlled randomness. He considers this concept essential for bringing music up to date with modern scientific thought. "A lot of composers are still exhibiting a mentality that comes from the eighteenth century," said Tipei. "It's an understanding of the world that can be described by Newton's mechanics. Everything is deterministic and rational. I think that our view of the world as a society has changed dramatically in the twentieth century. You have the relativity theory, quantum mechanics, and all the other developments in physics. Somehow this didn't fully trickle into the arts."

"I think that our view of the world as a society has changed dramatically in the twentieth century."

Quantum theory employs the mathematics of probability to investigate atomic and subatomic phenomena. This has brought randomness to science—something foreign to Newtonian methods of investigation. Tipei wants to incorporate this same idea in his music.

NCSA's CRAY X-MP/48 supercomputer is the essential tool for expressing the randomness Tipei desires. His music involves computations so lengthy that the CYBER 175 took 20 hours to complete one of his works in 1986. The CRAY X-MP system now accomplishes the same amount of work in 10 minutes. This advantage enables Tipei to shape a musical piece much more quickly. Just as the supercomputer provides scientists with a means of probing complicated systems in Nature such as thunderstorms, it also allows artists like Tipei the freedom to explore imaginary worlds of music—faster and in a more thorough way.

Tipei's music is called contemporary, but it shouldn't be confused with pop, rock, or new wave. To him these are just updated versions of an outdated musical philosophy. Any music that tries to tell a story using tonal chord progressions is outdated in Tipei's view, because these are analogous to Newtonian cause and effect. His music requires true randomness—something beyond human ability. " People are not very good at handling randomness," says Tipei, "because randomness is never truly random. We always bring in our prejudices and our conditioning."

Man and machine collaborate

When Tipei gets an idea for a work, his first step is to confine the piece within specific boundaries. He decides what types of instruments are to be played, how many, and a host of other musical constraints—along with specifications about time, pitch, timbre, dynamics, and instrumental effects. In his most recent work, a percussion ensemble entitled "Many Worlds," the list of constants and variables resulted in a data file 1 inch thick. MP1, the program that Tipei developed for composition, uses this data as input. A wide range of musical possibilities exists within these limits. Once Tipei begins to run a program, the end result is beyond his control.

Tipei uses the analogy of a boiler to describe some aspects of his music. "What happens to a boiler when you put a flame underneath? The water starts heating up, some molecules evaporate, and it either explodes or you control the thing. The idea is that you know the overall behavior of the boiler, although nobody is going to be able to tell you what a particular molecule is going to do in the next two seconds. In the same way, one can build very large aggregates of sounds—where the overall shape is described precisely—but the particular sounds are not controlled by the composer."

In this analogy, the cloud of steam is the piece. Its size, shape, temperature, and chemistry are determined by the composer through his design of the boiler and the materials he places inside. Tipei builds and stokes his boiler on the computer using a set of musical constraints. The resulting composition is made of notes chosen by the computer. The notes are like the randomly moving molecules in a cloud of steam, yet none of them violate the constraints imposed by the composer. When the notes are played, patterns begin to emerge in spite of their random origin—patterns reminiscent of many occurrences in Nature. For example, Tipei's work "Maiden Voyages" begins softly and gradually develops patterns that climax and then diminish—like a flower that buds, opens to a full bloom, and

***Music** continued on page 14*

Music continued from page 13

withers or like the symphony of sounds encountered on a trip into the jungle.

Once Tipei has built the framework for a musical piece, he triggers the program with a nine-digit "seed" number. [Any nine-digit number.] When the computer completes its run, Tipei is left with the numerical equivalent of a musical composition. He must decode it to get a musical score. Decoding used to be done by hand, and it took months to produce the score for one piece. Now Tipei is overseeing development of a program in the computer music project at UIUC's School of Music that will produce a score automatically from the supercomputer's numerical output. It will eventually enable Tipei to run different versions of a composition in a very short time.

Manifold compositions

Computer speed is important to Tipei, because he wants each computer run of an individual piece to be played only once. He calls this idea "manifold composition." It represents another way he expresses randomness. Just as events in Nature are never precisely duplicated, so Tipei desires that his pieces are never exactly the same each time they are played. For example, if a person decided to attend two concerts featuring Tipei's piece "Many Worlds," he/she would not hear the same music at both concerts—and that would not be because a musician slipped up. The person would hear two "variants" of the same music, the result of two different seed numbers being fed into the program that produces "Many Worlds" on the supercomputer. With a nine-digit seed number to work from, Tipei has a very large number of possible variants of each piece. He makes a separate computer run for each concert, usually using the date of the concert as the seed number. While the resulting variants sound similar, they are not precisely the same.

Until the advent of the supercomputer, the idea that a large musical composition might be played once and thrown away was never workable. No composer wanted to go to such effort for such a fleeting reward. Now Tipei is not only looking at this idea but beyond to other possible uses of the supercomputer in music. He divides the uses of the computer into two categories. First is the computer as collaborator, or the field of computer-assisted composition. This is the use that Tipei is exploring presently. The computer helps him write the music, but it is performed with traditional instruments and/or live voices. The second category is the computer as instrument, or the field of sound synthesis. Tipei hopes to explore this area in the near future and eventually combine it with computer-assisted composition. Another project which Tipei would like to devote his time to is finding effective ways to represent complex structures and data through sounds as a complement to scientific visualization.

Supercomputing in music education

Tipei spent much of his summer learning more about NCSA's facilities and the capabilities of its supercomputers. He attended three NCSA summer workshops: the 1989 Summer Institute organized by Alan Craig, graphics consultant; the Supercomputer Education Workshop conducted and organized by Dr. Nora Sabelli, senior research scientist; and the Massively Parallel Computing Workshop organized by Michael Welge, associate director of Applications.

At the sessions, Tipei found out about the newest advances in supercomputing technology. This new information, Tipei is discovering, will help him as a composer as well as in his teaching. As a result of Sabelli's Supercomputer Education Workshop, this fall Tipei is teaching a seminar entitled "Musical Applications on Supercomputers."

In addition to computer-assisted composition, other topics in Tipei's seminar are visualization of music, automatic music notation, nontraditional sound synthesis methods, and aural rendition of complex structures and data (ARCS).

NCSA's Education Program provides access to the supercomputer for Tipei and his students. Tipei is pleased with the interest the seminar has received. He foresees the seminar developing into an interdisciplinary meeting ground where musicians, computer scientists, engineers, visual artists, and students from other fields can exchange ideas and work on common projects relating to music. He would like to see scientists exploring their artistic skills and artists growing in their scientific understanding.

Sever Tipei.

Performing via the Crays

Tipei presented a paper on manifold compositions at the 1989 International Computer Music Conference at Ohio State University in Columbus, OH on November 3. (NCSA cosponsored the 1987 conference which was held at UIUC.) He discussed how he produces multiple variants of a piece with NCSA's CRAY X-MP/48 supercomputer. One week later, Tipei presented a similar paper at the New Music and Art Festival at Bowling Green State University in Bowling Green, OH.

On February 21, 1990, the UIUC Percussion Ensemble will perform "Many Worlds" at Krannert Center for the Performing Arts.

Another of Tipei's works, "Cuniculi," has been released by Centaur Records on a compact disc entitled *Computer Music from the University of Illinois.* ▲

A new affiliate explores outer space

by William Dwyer, Graduate Student Writer

For several years Richard White has been using supercomputers to run simulations of stellar dynamics of galaxies to understand their structure and evolution. Until recently he has had to limit himself to "smaller dimensions," he says, due to memory limitations of the computers available to him. Now he has access to the "huge amounts of memory" of the CRAY-2 supercomputer for doing the phase space calculations required for his simulations.

White is a researcher at the Space Telescope Science Institute in Baltimore, MD, one of the newest members of NCSA's Affiliates Program. Besides his own research applications, White arranges supercomputing time for other members of the institute. There are about 80 Ph.D. astronomers at the institute who work on their own projects and space telescope projects. About 30 groups or individuals have already expressed interest in the program, and White has received about 20 proposals for time on NCSA's supercomputers.

"Once things get going and people see that it's pretty easy to do, there will be a lot more interest to use [NCSA's supercomputers]," White explains. "Most [researchers] have been put off by the idea of applying for time and computing remotely." Researchers at the institute had been running a lot of long programs on VAXes and Suns. White says,"We're hoping to encourage people to move their work to the bigger machines." He expects many of them to do just that because the arrangement for using NCSA's facilities is an "easy mechanism for people to work with."

Benefits of the program

Those researchers who have not used supercomputers can become familiar with the system. Some of them will take advantage of their time to experiment with various operational techniques, such as a proposal to explore algorithms of artificial intelligence expert systems for scheduling experiments on the space telescope.

Proposals for time on NCSA's supercomputing system include simulations on stellar dynamics like White's. Another project will study the dynamics of solar nebulae to understand the evolution of solar systems. A

New Affiliate *continued on page 22*

New NCSA affiliates

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Peoria, IL
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Phone: (309) 677-2766

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Baltimore, MD
Glenn Dorsey
(301) 333-7725

Montana State University
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Allen Porter
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Prairie View A&M University
Prairie View, TX
S. T. Koay
Department of Electrical Engineering
(409) 857-3923
and
Kwang Paick
Department of Computer Science
(409) 857-4546

An undergrad's perspective on New User Training

by Linda McDonald, Physics Professor, North Park College

Deb Sunberg, a junior physics major at North Park College in Chicago, is currently working on a research project with Nora Sabelli, NCSA senior research scientist, and Linda McDonald, physics professor at North Park. The goal of their project is to produce graphic representations of molecular orbitals that were calculated using a configuration interaction based approach for various unstable resonances. To prepare for the project, Sunberg recently attended New User Training at NCSA.

Before attending training, Sunberg had experience on a VAX 11/750 programming in Pascal and on Macintosh SEs and IBM PCs using packaged routines. The New User Training was her first exposure to supercomputers and the UNIX operating system.

At North Park—an NCSA academic affiliate, Sunberg works as a student consultant in the new computer lab which is open 20 hours daily for faculty and students. She helps students with their programming and PC problems. With her New User Training, Sunberg is also consulting with students and faculty who are learning to use the Crays.

Outside class, Sunberg is active as president pro tem of the Society of Physics Students and president of the Dorm Council and Resident Women's Council. She is also very active in campus religious activities. She is from a small town—Red Oak, IA.

"Wonderful" people, "great" experience

After returning to North Park College, Sunberg commented about New User Training:

Training *continued on page 16*

***Training** continued from page 15*

Deb Sunberg (Credit Jim Foley).

“The New User Training was interesting to me as a completely new user of the supercomputer. At times I was overwhelmed by the amount of information. I’m sure that the people with previous experience in large-scale programming got a lot more out of the sessions than I did. But I learned a lot!

“As a student, it was very difficult to manage classes when I had to miss four days. I was not only missing out on the lectures but also on the homework time. Even though I had gotten assignments from my professors before leaving, I really didn’t have time to work on them while I was there. I tried to take advantage of the lab time on the Crays from 6:00 to 9:00 in the evenings, which meant that I had basically spent the day from 8:30 a.m. to 9:00 p.m. in training. Maybe it’s just me, but after a day like that I really didn’t have the energy or mental capacity to do work for my classes.

“I realize it sounds as though I don’t have anything positive to say about the session. This is not true! The staff was very helpful and more than willing to give of their time. I will admit that I felt a little overwhelmed to realize that most of the others taking the classes were in industry and had their master’s degrees, if not their Ph.D.s, and there I was—‘Hi, I’m an undergraduate.’ I was pleasantly surprised to find the people were friendly and didn’t look down on me

***Training** continued on page 24*

Industrial Program

Jeff Simon (left) and John Patten (right).

Easing industrial partners’ paths

by Stephanie Drake, Publications Editor

John Patten and Jeff Simon were recently named assistant directors of the NCSA Industrial Program. They are responsible for monitoring the full-partner agreements and stimulating their success. Currently NCSA’s six full industrial partners are Eastman Kodak, Amoco, Eli Lilly, Motorola, FMC, and Dow Chemical.

John Stevenson, associate director of the Industrial Program, explains, “The full industrial partner company responsibilities will be split between John Patten and Jeff Simon, each assigned to specific companies. They will be essential to the implementation and ongoing operations of the Industrial Program’s full partners.”

Stevenson and NCSA Director Larry Smarr are primarily responsible for the diplomatic task of selling the program to industrial partners. Once a company becomes an NCSA industrial partner, the contract must be fulfilled so that the partnership benefits both the partner-institution and NCSA. While Simon says that he “advocates the spirit of the contract with each partner,” Patten nods in agreement. They concur that contracts must be mutually beneficial to partners as well as the center and that a successful Industrial Program is vital to accomplishing NCSA’s mission—particularly in strengthening the competitiveness of American industry.

Forming successful partnerships

Patten and Simon are committed to helping partners achieve their goals, and they agree that lots of thing are necessary to enable successful partnerships with NCSA. Partners come to NCSA to use the facilities and gain exposure to state-of-the-art technology. Patten explains, “We are not involved in directing partners’ projects. We may not even know what a project is, but we make sure the partner has all that’s needed to make its projects successful.”

Their commitment to the success of NCSA’s Industrial Partners Program is undeniable as they explain the services provided to partners which include:

- helping partners get to NCSA
- establishing the right workstation environment for each partner
- introducing company scientists to key people in each NCSA group
- keeping partners informed of what is happening in the center
- satisfying corporate requirements for security, accounting, administration, and training
- revisiting the agreement from time to time as changes (such as the installation of new equipment) occur at NCSA
- getting the appropriate NCSA services and tools to each partner
- reviewing technology, interpreting what is best for a particular partner
- helping partners get acclimated to an academic environment

Industrial consultants handle day-to-day projects while Patten and Simon make sure the partners' overall needs are being met. Jim Ferguson, Scott Piette, and Ilhan Dilber are industrial consultants.

Doing even more

As they become more familiar with their roles, Patten and Simon expect to travel to corporate headquarters and other sites, promote programs, discuss partners' problems, and look for improvements.

Simon states, "We need to concentrate on a training program—gearing it for industrial partners. We need to educate users in the use of new applications, concentrating on more flexible training so that scientists can come here for one or two days and go back to their corporations with something they can *apply*." Patten adds, "This is part of making things smooth, easy, and effective for our partners."

Simon explains, "Industrial scientists are focused on analyzing computational results—the speed and ease for solving large problems is a competitive advantage."

"We help partners enhance their competitive position in the marketplace," Patten joins in, "that's their bottom line."

A good match

"Our abilities are a good match. We complement one another. Jeff has the technical computer background," Patten says.

Simon quickly adds, "John brings us considerable management and training experience."

Patten spent most of his adult life in the US Navy. His assignments included command of a nuclear-powered, fleet ballistic missile submarine; director of officer training at the U.S. Navy Submarine School; executive officer of the navy's largest intermediate maintenance facility for nuclear submarines. After retiring from the navy, Patten served as director for nuclear training and emergency response for Illinois Power Co.; vice president and chief operating officer for Sublogic Corporation; and, most recently, vice president and general manager for Memory Storage Devices Inc. He earned a B.S. in Engineering from the U.S. Naval Academy, Annapolis, MD, and an M.B.A. from the University of New Haven in Connecticut.

Simon has been an NCSA consultant for three years, and most of that time he was an industrial consultant for Eastman Kodak. Before coming to NCSA, he spent two years with Analytic Services, a low-profile think tank in Washington, DC. He worked on CRAY-1 systems for three years at Lawrence Livermore National Laboratory prior to that. While at Livermore, Simon earned an M.S. in Computer Science at the University of California at Davis. He graduated from UIUC with a B.S. in Aerospace Engineering. ▲

Eli Lilly's FOCUS on molecular design

*by Sam Milosevich, Industrial Consultant**

Eli Lilly and Company's "FOCUS on Chemistry Using Supercomputers" was the first research application workshop produced by an industrial partner at NCSA. During a week in mid-August, 20 participating research scientists and research advisors learned to use the MACROMODEL molecular modeling system as a visual and computational tool to investigate chemical systems selected by the participants.

Professor Clark Still from Columbia University, originator of the MACROMODEL system, opened the workshop with a presentation on "The Philosophy and Essence of Macromodel." The workshop continued under the instructional guidance of Dr. Mark Lipton from the University of California at Berkeley and Dr. Jeff Howbert from Lilly Research Laboratories (LRL). Additional support was provided by Lilly staff from Scientific Information Systems and from the Supercomputer Applications and Molecular Design Department.

Facilities for the workshop provided by NCSA and Lilly mimic the standard DEC VAX/VMS scientific computing environment at the Lilly Research Laboratories. So the experience gained at FOCUS is totally applicable to continuing scientific computing efforts at LRL. Interactive graphics computations utilized Lilly's MicroVAX 3600 and the VAX systems at NCSA while large calculations were executed on the NCSA's CRAY-2.

Critical to the success of the workshop was the capability of obtaining computational results, from real calculations of immediate interest, while the instructors were available for consulting. Many scientists were eager to return to the laboratory to obtain experimental verification of the final results of the workshop computations.

FOCUS was a true "scientific bootstrapping" operation in which Lilly research scientists and systems analysts already trained by NCSA helped train other scientists.

The concept of the FOCUS workshops originated with Dr. John Wold, an executive director of Lilly Research Laboratories, and was organized by Dr. Riaz Abdulla, head of the Supercomputer Applications and Molecular Design Department at Lilly. Response to the first FOCUS was so great that Lilly plans to produce several more industrial research application workshops in a variety of areas.

* Currently Research Scientist, Lilly Research Laboratories

▲

Dave Thompson wins NCSA undergraduate award

by Mary Hocks, Technical Writer, Software Tools Development Group

In recognition for his distinguished service to NCSA, Dave Thompson is this year's recipient of the NCSA Undergraduate Employee Scholarship Award. Thompson is a student programmer/project leader in the Software Tools Development Group (STDG), formerly Software Development Group (SDG).

Thompson has been programming for NCSA since November 1985. In May 1990 he expects to graduate from UIUC with two degrees—a B.S. in Computer Science and a B.A. in Psychology with emphasis on human-computer interaction.

NCSA established the Undergraduate Employee Scholarship Award in 1988 to acknowledge outstanding efforts by an undergraduate member of the staff. The scholarship provides an undergraduate NCSA employee with tuition at UIUC. Gaige Paulsen, then working in SDG, was last year's award winner [see ***access***, September-October 1988].

Developing prize-winning software

Thompson's accomplishments and awards demonstrate the high quality of his work at NCSA. He is currently project leader for the development of NCSA X Image, a versatile and comprehensive color imaging and data analysis software tool designed to run under the X Window System [see ***access***, July–August 1989]. His program won acclaim at the UIUC's annual Engineering Open House last spring. Thompson entered the prerelease version of NCSA X Image in the "Original Research by Undergraduates" category and placed first [see ***access***, May–June 1989].

Thompson points out that NCSA X Image is on the cutting edge of X software because it was designed specifically as a "generic tool" for users of large workstations. "Scientists needed visualization tools for many platforms. Because it is a generic tool, X Image will run on virtually any platform that supports X.

"The biggest challenge," he explains, "was that X Image was the first program for X Windows developed at NCSA. Developing it was a path to learning X Windows and producing something in the meantime."

A participant in a number of X Window conferences and exhibitions, Thompson keeps STDG staff members well informed by "watching developments and keeping us up-to-date on what's going on in the X Window world."

NCSA X Image for X Window Systems

At Xhibition '89 held recently in San Jose, CA, Thompson gave a slide presentation/demonstration of NCSA X Image as a scientific visualization tool that takes full advantage of the newest X Window software and state-of-the-art hardware.

NCSA X Image combines the functionality of the recently released Macintosh tools—NCSA DataScope, NCSA Image, and NCSA PalEdit—into one application that runs on any system supporting the X Window System (that is, a Sun, DEC, or IBM RT workstation). Features of this application promote advanced data analysis and experimentation.

NCSA X Image allows users to view and manipulate data values, including datasets calculated on the CRAY X-MP/48 or CRAY-2, and digitized pictures. The application reads datasets from Hierarchical Data Format (HDF), raw raster, and raw palette files. It displays a dataset as real data values in spreadsheet form, as full-color Cartesian or polar raster images, or as a contour or shaded data plot. Image manipulation features include pixel or bilinear interpolation expansions and compressions and animation of multiple-color raster images.

Dave Thompson.

NCSA X Image helps users determine which colors are mapped to real data values. One can compose palette colors and perform global operations such as rotating, flipping, smoothing, or "fiddling" the palette. X Image features color histograms of the frequency distribution of data.

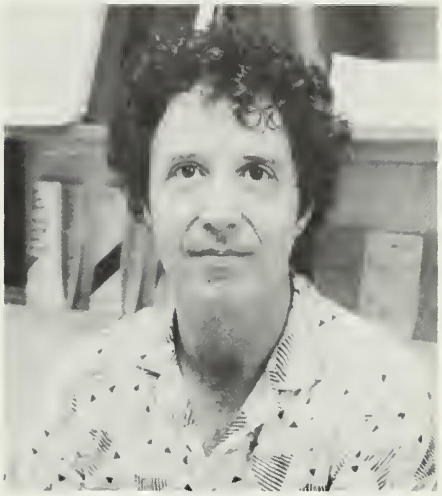
Well done, Dave!

Although the program is relatively new and still awaits its first full release, Thompson expects NCSA X Image to have a wide distribution and user base comparable to other NCSA visualization tools. Approximately 70 users have obtained the beta release version of the software since August 1989. Thompson is currently arranging to have NCSA X Image distributed on the X11 Release 4 tape bundled with X Windows.

NCSA X Image has pioneered NCSA X Window software for an increasingly popular environment. Thompson's commitment to X Windows helps give the Software Tools Development Group a strong presence in an exciting new area of software development.

Congratulations, Dave, from all your colleagues at NCSA! ▲

Left. NCSA staff mingled with attendees during the lunch breaks for user feedback.



User Group Meeting

by Fran Bond, Technical Editor

Approximately 42 people attended the second annual User Group Meeting held October 23 through 25 at the Beckman Institute. In his welcoming remarks, NCSA Director Larry Smarr noted that supercomputing users at the five NSF centers have grown from 200 to 20,000 over the five years since the centers were formed. At dinner the first evening of the conference, John Kogut—one of NCSA's earliest users and UIUC professor of physics—spoke of the drive for faster computers in his keynote entitled "RISCy Business: The Future of US Supercomputing." For two days, attendees heard an overview of NCSA's accomplishments, services, and scientific programs by members of the staff. At lunch both days and at the question and answer session with Deputy Directors Karl-Heinz Winkler and Jim Bottum, users gave staff members feedback about NCSA operations. Visitors toured the Beckman Institute for demonstrations of the Renaissance Experimental Laboratory and the Connection Machine. Tutorials on NCSA software, UNICOS shell scripts, and autotasking concluded the meeting. ▲

Above right. In his keynote speech, John Kogut addressed the "RISC (reduced instruction set code) revolution" in machine architecture. Kogut predicted that over the next decade this revolution will lead to an increase in the development of massively parallel machines as well as the production of desktop workstations equivalent to today's Cray supercomputers.

Above. Attendees enjoyed sending electronic mail to their home sites from the Beckman Institute.

Center cache

by Fran Bond, Technical Editor

Towards a digital library

Dr. Bruce Schatz, developer of a unique networked digital library system at Belcore and now continuing this work for the Computer and Genomic Systems Laboratory at the University of Arizona, spoke to the NCSA staff in early October. This is the first in a series of presentations to educate NCSA staff members about Director **Larry Smarr**'s vision for implementing a networked digital library of information at the center.

"Telesophy: Towards Worldwide Information Spaces" was the title of Schatz's talk. Schatz defines telesophy as "all the world's knowledge with transparent access to it." Using the concept of a library as a metaphor for a distributed multimedia knowledge repository, Schatz described the technology and architecture needed to make such an "information space" (or an electronic library containing a special group of knowledge) a reality. He emphasized the necessity for high-speed access. To demonstrate the system's design and capabilities, Schatz concluded his lecture with a lively demonstration of the setup used by molecular biologists at the Arizona lab.

Recent personnel changes

Karl-Heinz Winkler, deputy director for Science, Technology, and Education, recently announced the following appointments:

Daniel Alpert is associate director for Faculty Programs. In this newly created position, Alpert will provide leadership in facilitating and strengthening faculty-related collaborative projects and programs that relate NCSA to activities of the Beckman Institute and the University of Illinois at large. He will formulate NCSA policy for faculty programs and faculty relations and establish budgetary requirements. Alpert will have direct responsibility for implementing policy, overseeing collaborative projects, arranging project reviews, and managing the NCSA budget for these programs. He will coordinate the efforts of the Offices of the Deputy Director for Science, Technology, and Education and the Director of NCSA in supporting the progress of ongoing collaborative projects and the development of new initiatives in research and education.

Lex Lane is now associate director for Systems and Software Development. Managers of the following groups will report directly to him: Networking Development and Telecommunications, System Integration, Software Tools Development, and Visualization Development and Services. This area serves a key role in identifying and implementing the introduction of new technologies to the NCSA computational environment. Lane will work with managers of the above groups to coordinate the groups with the Deputy Director for Science, Technology, and Education in establishing plans and policies, budgetary responsibilities, and implementing effective procedures for interacting with other groups. In addition, Lane will manage the operational aspects of the deputy director's office in the deputy director's absence.

Scott Lathrop is associate director of the Academic Program. He is administering the programs that serve NCSA users to increase representation and advocacy of academic researchers. Under his direction, several new programs are being initiated to work with and support the academic community. Lathrop organized the orginial consulting and user services groups at NCSA. He also organized the first intercenter working group on user services and is recognized as a national leader in center collaboration.

Michael Smith has been promoted from assistant director to associate director for Computer Operations and System Administration. In this position, Smith will continue to provide leadership for all aspects of computer operations and system administration of NCSA's central facility, the network, distributed workstations, and the numerical laboratory. Smith will also continue to be in charge of facilities design and engineering at NCSA. He will be responsible for formulating and implementing policies and procedures in his areas of responsibility as well as ensuring smooth day-to-day operations.

Michael Welge is associate director for Applications, a position he has held on an acting basis since July 1989. Welge will continue to provide leadership in facilitating the efficient coupling of scientific and engineering applications to NCSA's rapidly changing technological base. Welge is responsible for the oversight of a large number of application teams involved in scientific research; in the evaluation, installation, and maintenance of application software; and in user consulting. In addition, he oversees the development of new approaches and curricula for education in computational science.

Alpert lecture

NCSA cosponsored The 1989 Daniel Alpert Lecture together with the Beckman Institute for Advanced Science and Technology and other campus units in mid-October. Lewis M. Branscomb spoke on "The Wellsprings of American Technology: Balancing Public and Private Interests in Science and Technology"at the Beckman Institute Auditorium.

Branscomb is Albert Pratt Public Service Professor and director of the Science, Technology, and Public Policy Program at the John F. Kennedy School of Government at Harvard University. He addressed current US policies in science and technology and outlined how they affect industry and higher education as well as government research and development efforts in science and technology.

Alpert has been a member of the Beckman Institute's Program Advisory Board from its beginning.

Cox honored

Donna Cox, UIUC assistant professor of art and design and adjunct professor at NCSA, was named a University Scholar recently at the University of Illinois Foundation's 54th annual meeting. Director of the Renaissance Experimental Laboratory which was dedicated at the Beckman Institute last April, Cox is a principal investigator and project leader at NCSA who developed and initiated the Renaissance Teams Approach to collaborative scientific investigation. ▲

***Allocations** continued from page 6*

David A. Russell, University of Washington, *Vortex Generator Aerodynamics*, CRAY X-MP/48 and CRAY-2, 90 SUs.

David N. Ruzic, University of Illinois at Urbana-Champaign, *Interaction of Ions and Atoms with Surfaces*, CRAY X-MP/48, 25 SUs.

John Slattery, Northwestern University, *The Physics of Moving Common Lines*, CRAY X-MP/48, 100 SUs.

John D. Stack, University of Illinois at Urbana-Champaign, *Lattice Field Theory on a Supercomputer*, CRAY X-MP/48, 135 SUs.

James C. Swihart, Indiana University, *Electronic Properties of Alloys*, CRAY-2, 226 SUs.

Paul R. Woodward, University of Minnesota, *Simulation and Visualization of Fluid Flow in 3D*, CRAY-2, 1600 SUs.

Robert E. Wyatt, University of Texas, *Quantum Reactive Scattering via the Log-Derivative Version of the Kohn*, CRAY-2, 300 SUs.

Small Allocation Committee Meeting—September 12, 1989

Principal investigators and their approved projects are as follows:

M. Quinn Brewster, University of Illinois at Urbana-Champaign, *Solid Rocket Motor Internal Flowfields*, CRAY X-MP/48, 75 SUs.

S. J. Chang, University of Illinois at Urbana-Champaign, *Quantum Mechanics of Classically Chaotic Systems*, CRAY-2, 5 SUs.

B. T. Chao, University of Illinois at Urbana-Champaign, *Unsteady Motion in Pipe Flow of Dense Gas-Solid Suspension and Modeling*, CRAY X-MP/48, 26 SUs.

Michael Chen, University of Illinois at Urbana-Champaign, *Enhanced Residual-Based Iteration for Incompressible Fluid Flow and Heat Transfer*, CRAY X-MP/48, 30 SUs.

Michael Chen, University of Illinois at Urbana-Champaign, *Influence of Convection on Material Processing Techniques Involving Melting and Resolidification*, CRAY X-MP/48 and CRAY-2, 15 SUs.

Robert Clayton, California Institute of Technology, *Mantle Dynamics*, CRAY-2, 80 SUs.

Freddie J. Davis, Texas A&M University, *Finite Element Method and Large Eddy Simulation for Turbulence Modeling*, CRAY-2, 75 SUs.

Dana Dlott, University of Illinois at Urbana-Champaign, *Vibrational Heating by Shock Wave*, CRAY X-MP/48, 80 SUs.

Ronald Dougherty, Oklahoma State University, *Radiative Transfer within Participating Media*, CRAY X-MP/48, 10 SUs.

David E. Ford, University of Washington, *Tree and Stand Growth Assessment and Modeling of the Effects of Pollutants on the Physiology and Growth of Trees*, CRAY X-MP/48, 70 SUs.

Randall LaViolette, Rockwell International, *Phase Transitions at Negative Pressure*, CRAY X-MP/48, 40 SUs.

Ki D. Lee, University of Illinois at Urbana-Champaign, *Modeling and Analysis of Vortex Dominated Flow-Fields*, CRAY-2, 96 SUs.

S. W. Lee, University of Illinois at Urbana-Champaign, *RCS of Complex Objects*, CRAY X-MP/48, 80 SUs.

John McLaughlin, Clarkson University, *Direct Numerical Simulation of Aerosol Motion in the Viscous Wall Region of a Turbulent Shear Flow*, CRAY-2, 20 SUs.

Roger A. Pielke, Colorado State University, *Impact of Regional Flow Patterns on Mountain / Valley Thermally Induced Mesoscale Circulations and Application of the Receptor-Oriented Approach in Mesoscale Dispersion Modeling*, CRAY-2, 50 SUs.

Andrzej Rajca, Kansas State University, *Highly Charged HeC Clusters, Hypervalent Carbon*, CRAY-2, 20 SUs.

***Allocations** continued on page 22*

September allocation statistics

	SAC meeting		PRB meeting	
Number of proposals	28		36	
CRAY X-MP only	14		11	
CRAY-2 only	12		16	
CRAY X-MP and CRAY-2	2		9	
Fully allocated	17		16	
Partially allocated	6		17	
Deferred	5		3	
	X-MP	**CRAY-2**	**X-MP**	**CRAY-2**
Hours requested*	571	663	6185	10757
Percent allocated^	90%	53%	52%	76%

* These figures reflect what is allocated for the coming year only. They do not include service units for years 2 and 3 of multiyear requests.

^ Some allocations were deferred pending requests for additional information from researchers. These will be acted on prior to the next meeting if possible. Deferred allocations are not included in these figures.

***Fault** continued from page 3*

tools this could have been a major 'oops' persisting for months before being detected by one of my colleagues. With these tools, such problems are easily and routinely detected."

Lyzenga's account shows that he uses DataScope and Image as data analysis tools as well as code development tools.

Completing the process

NCSA DataScope and Image enable the researchers to generate images from their data. Lyzenga explains the importance of using NCSA PalEdit to further interpret their results. "In the work I've been doing on the San Andreas Fault, [it's] characterized by lots of things happening very rapidly in a zone where things are interesting. That is, near the fault things are changing very rapidly; far away from the fault things tend to be very smooth and uninteresting. It's kind of a challenge to figure out how to display the data in such a way that it emphasizes the salient features of interest while not being so busy that it gives you sensory overload. Using PalEdit ... [has] allowed me to tweak and optimize palettes in such a way that it gets the point across."

As a final step, he displays the images and their palettes in NCSA Layout to make presentation slides, and through the program's animation option, make videotapes.

The images shown on pages 1 and 3 are taken from the dataset included on the Apple '89 CD. They represent the accumulation and release of strain on a strike-slip fault that cuts through an elastic/viscoelastic earth model. Starting from page 1, they show the migration of stress at successive times in the earthquake cycle. The range of stresses represented in these images is from 0 to 100 MPa [1 MPa = 1 MegaPascal = 10 bars].

Accessing insights

Increased computer power from the use of both Crays, parallel processing from the CRAY-2, and NCSA tools has allowed Lyzenga accessibility to "insights that weren't possible before. If it had been possible to look at the reams of data that I got three years ago," he states, "I may have been able to make some of the same conclusions that I'm making now."

Lyzenga summarizes the helpfulness of NCSA's Scientific Visualization Software Suite as he talks about his current work. "I've been going through a fairly lengthy process of refining the models and discovering what was right or wrong about the old ones and how to make them better reflections of what might be actually going on on the real Earth. ...Doing that over the last two to three years, it's been roughly equal parts of refining the science and refining the technique. Sometimes I would find that what was wrong with my models had to do with wrong-sized time steps or that I was integrating something in the wrong order. In those cases, I had to fix up a numerical detail. Other times I would find out that my numerics were just fine, but that my physics needed to be better.

"So it's been about 50/50—both physical insights and techniques. I would have to say that using the visualization software has been a real revolution. Being able to turn around a result and see the content of it in a matter of at most hours—instead of days, as we used to work—has greatly accelerated the pace of progress in this work."

Currently Lyzenga is documenting his latest work on the San Andreas Fault, and Raefsky is collaborating with him while working on semiconductor device simulation at Stanford. ▲

***New affiliate** continued from page 15*

third project plans to probe the structure of stars by analyzing a large quantity of data from high-speed photometric observations of stars like the Sun.

According to White, researchers doing data analysis can benefit from NCSA's visualization tools. They will take advantage of the capability to "look at data in a lot of different ways" by producing an image that can be manipulated. He states that a lot of modern instrumentation is now producing three-dimensional data—a data cube—for which visualization is a sophisticated and useful analytical tool.

White found out about NCSA's Affiliates Program from Ronald Allen, former chair of the Department of Astronomy at UIUC. Allen now heads the computing division at the Space Telescope Science Institute and is a visiting professor from the Space Telescope Science Institute to the Beckman Institute.

Janice Knapp-Cordes, assistant coordinator of Training, says the institute is one of the most sophisticated groups in the Affiliates Program. Knapp-Cordes spent two days at the institute in July orienting users to NCSA's facilities. Several members of the institute staff volunteered to be consultants to help others use NCSA's facilities.

White currently budgets modest amounts of time on the system for interested users. If their results on the system are conducive to doing so, he will help them apply directly to NCSA for additional computing time. ▲

***Allocations** continued from page 21*

Roger H. Rangel, University of California–Irvine, *Liquid Waste Incineration*, CRAY X-MP/48, 10 SUs.

Umberto Ravaioli, University of Illinois at Urbana-Champaign, *Computational Electronics Laboratory*, CRAY X-MP/48, 20 SUs.

Walter A. Robinson, University of Illinois at Urbana-Champaign, *The Generation of Extra-tropical Low-Frequency Variability,* CRAY X-MP/48, 10 SUs.

Nancy E. Westcott, Illinois State Water Survey, *Precipitation Augmentation for Crops Experiment (PACE)*, CRAY X-MP/48, 7 SUs.

Bob Wilhelmson, University of Illinois at Urbana-Champaign, *Computational Fluid Dynamics*, CRAY X-MP/48, 30 SUs. ▲

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FAX (217) 244-1987

Orders for Documentation and Publications
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(217) 244-4130

Cray Operations
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***Training** continued from page 16*

for my lack of education. In fact, I was received with almost the exact opposite response! Since people realized I hadn't had much education, they were even more helpful to me.

"Overall, I felt that I had a very good experience at the New User Training. I am sure that once I have a chance to actually work on the computer, what I learned will make even more sense to me. Despite the information overload and missing class, the experience was great. The people were wonderful and made me really feel like I belonged there."

North Park College, a recent academic affiliate of NCSA, is a four-year, Christian liberal arts college with a strong commitment to quality undergraduate education. With a full-time enrollment of approximately 1,000, North Park has a large number of Merit Scholars. In recent years, the college has had a 90 percent acceptance to medical schools from its pre-med program. The college was selected as one of the top ten regional liberal arts colleges in a recent *U.S. News and World Report* survey. ▲

data link Contents

- Hot tips and topics
- Adding directory changes to your UNICOS prompt
- A quick look at the Model CM-2 Connection Machine
- BCS updated to Version 11 on the CRAY X-MP system
- GLIM available on the CRAY X-MP system
- SPARSE package on the CRAY X-MP system

If you want to receive a copy of the current ***data link***, contact Debbie Price at (217) 244-4130

Connection Machine access

The Connection Machine is now in a friendly user mode. The Friendly User Period will last through December, 1989. To gain access under the Friendly User Program, please contact Michael Welge at the addresses opposite (see "Contacts"). Include a description of your plans and any previous experience on a Connection Machine. Time will be allocated through the standard process used for the Cray systems.

Operating schedule for the Connection Machine

Development time: 7 a.m. to 7 p.m. During this period, your code will be disconnected after 5 minutes if someone else is waiting to get access to the machine. Otherwise, execution will continue until the next user connects to the CM-2.

Production time: 7 p.m. to 7a.m. Users may use the online schedule program to reserve production time. (This operating schedule is subject to change based on experience and feedback from the user community.)

Calculation of service unit charge

One hour of time on the Connection Machine will be charged one service unit. During development time, connect time on the CM-2 will be charged. During production time, time reserved will be charged—regardless of lack of use of the machine.

Documentation

Documentation may be ordered from Thinking Machines Corporation, 245 First Street, Cambridge, MA 02142. Available manuals are listed in the latest issue of the NCSA *Technical Resources Catalog.* To obtain a catalog, contact Debbie Price at (217) 244-4130.

Training schedule

Training dates for the CM-2 will be Nov. 30–Dec. 1 at NCSA. Contact Kendra Reasor for details (see "Contacts" below).

Contacts

For friendly user time, contact Michael Welge, mwelge@ncsa.uiuc.edu or call (217) 244-1999.

For allocation of time, contact Patricia Wenzel, User Administration, pwenzel@ncsa.uiuc.edu or call (217) 244-0074.

For training information, contact Kendra Reasor, kreasor.ncsa.uiuc.edu, or call (217) 244-1100.

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K

This document contains index entries for the 1989 *access* newsletters. The three numbers used for the entries and subentries indicate the volume, issue, and page number(s) of the citation, in that order. For example, 3.4.6–7 means that the entry is in volume 3, issue 4, pages 6–7 of the newsletter.

This index is in the /usr/local/doc directory on the CRAY X-MP/48 and CRAY-2 systems. You can view the index, using the UNICOS file pager more, by entering:

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Center Activities

NCSA—the first five years

"...We propose the creation of a Center for Scientific and Engineering Supercomputing at the University of Illinois. The Center is meant to be a model of a new type of dedicated basic research facility in which large-scale problems of heretofore intractable complexity, in a wide variety of disciplines, can be successfully attacked. The Center will provide a focal point for bringing together innovative scientists, engineers, computer designers, and algorithm developers. They will work in a fully equipped, well balanced facility. ...The interaction of these talented users, combined with unprecedented amounts of computational resources per investigator, should lead to major advances in a number of frontier research areas. ...We believe that the proposed Center will have a dramatic impact on basic research in the United States."

—from "PROPOSAL: A Center for Scientific and Engineering Supercomputing" by Larry Smarr (Astronomy); John Kogut (Physics); David Kuck (Computer Science); Robert Wilhelmson (Atmospheric Sciences); Peter Wolynes (Chemistry); Karl Hess (Electrical Engineering); Thomas Hanratty (Chemical Engineering); Robert McMeeking (Theoretical and Applied Mechanics), November 1983. This proposal led to NCSA's founding in February 1985.

Beckman Institute, home of the Interdisciplinary Research Program. (Photograph © Larry Kanfer, Champaign, IL)

"[Computational science] is like science fiction, and we're doing it regularly [at NCSA]. ...What we have here is not the chance of a lifetime, but of a generation."

—from speech to NCSA staff by Larry Smarr, Director of NCSA, November 1989.

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Abbreviations

CRI	Cray Research Inc.
CSRD	Center for Supercomputing Research and Development
IRC	Interdisciplinary Research Center of NCSA
NCSA	National Center for Supercomputing Applications
NSF	National Science Foundation
UIC	University of Illinois at Chicago
UIUC	University of Illinois at Urbana-Champaign

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Catching Smarr fever

by Kathleen Robinson, Science Writer

Left to right: Jim Bottum, deputy director; Larry Smarr, director; Karl-Heinz Winkler, deputy director; and Mike Norman, research scientist. (Credit: Wilmer Zehr)

Just over five years ago, in August of 1984, reporters and news teams crowded the large board room at the National Science Foundation in Washington, waiting for an announcement of the Phase II competition for national supercomputing centers. NSF's Phase I approach had been to buy time for researchers on existing machines, but the intent had always been to establish national centers. Now that time had arrived.

NCSA Deputy Director Jim Bottum, then an associate program director at NSF, recalls the scene at the announcement. "It was standing room only. People were being turned away—and this is at NSF, which is not usually in the spotlight. The excitement was just tremendous. Researchers had been starving for access to supercomputers, and here was their chance. By the deadline two months later we had received 22 proposals totaling over $1 billion. We had three different review passes, conducted some site visits, and concluded with several proposals being rated 'excellent.' The difference between these and the fairly large number of proposals rated 'good' was that the former group showed vision for the way the program should be implemented, as well as technical competence. By December we had the proposals reviewed, documented, tabulated, and ready for presentation to the advisory committee. Announcements of the awards were made in February of 1985, just six months after the solicitations were sent out."

During this time, the NSF budget request was before Congress, a request for $20 million. Recalls Bottum, "Congress was very interested in the program and solidly behind the Centers concept, as evidenced in their doubling of the NSF request to $40 million."

In an unprecedented move, says Bottum, NSF "announced the awards before they were made, simply to get the congressional heat off our backs—there was so much national interest. We had the directors of the new centers come to Washington to speak at the announcement. Larry Smarr stood up there and said he felt the country had been fighting with one hand tied behind its back, but now this program would cut the ropes."

***Smarr** continued on page 4*

Milestones at NCSA

1983	Grant proposal submitted to NSF
1984	Congressional hearings and funding of national program
	Enhanced proposal to NSF
	National competition for NSF centers announced
1985	NCSA selected as one of three national supercomputer centers (along with SDSC and JVNC)
	NCSA established with NSF grant
	Computing Applications Building (CAB) occupied for first time
	CRAY X-MP/24 system delivered to Astronomy Building
	First file shipped from Apple Macintosh to CRAY X-MP/24 system
	Large Scale Scientific Computing Product Development Grant from IBM
	First visiting scientists use the CRAY X-MP/24 system
1986	NCSA opened to the national community
	NCSA held first Summer Training Institute
	Kodak became first member of NCSA's Industrial Program
	Advanced Visualization Facility for Computational Sciences designed
	CRAY X-MP/48 system installed

Milestones at NCSA

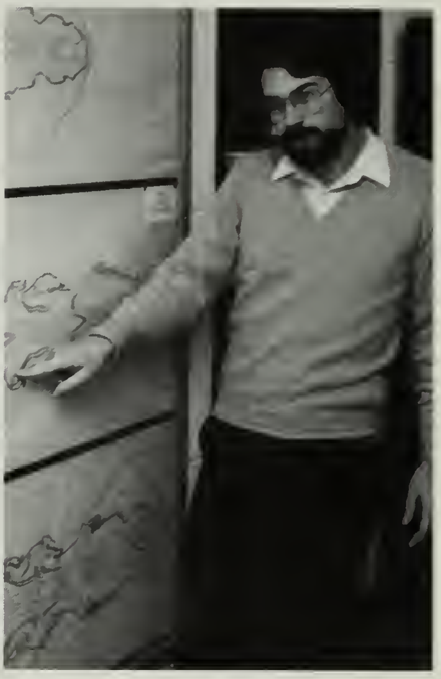
1986 *(contd.)*	Joint Peer Review Board established with Pittsburgh Supercomputing Center
	NSFNET 56Kbps backbone installed
	Sun Microsystems created Sun Room in CAB with donation of 8 Sun-3/160 Workstations (color) with graphics hardware
1987	Interdisciplinary Research Center officially opened to visitors through Visitors Program
	Apple Computer Inc. donates Mac Pluses and SEs for Training and Affiliates Programs
	Academic Affiliates Program announced
	NCSA took over facilities management from CSO
	Amoco became NCSA's second industrial partner
	NCSAnet established
1988	Eli Lilly joined Industrial Program
	Motorola joined Industrial Program
	100th employee hired in May
	NCSA held first User Group meeting
	CRAY-2S/4-128 system installed
	NSFNET upgraded to T1 bandwidth

***Smarr** continued from page 3*

Smarr *had* been fighting, for several years, to improve researchers' access to supercomputers. When Smarr completed an astrophysics doctorate in 1975, his advisor told him to get top-secret clearance so he could continue his black hole research in the national labs. At the time, these were the only U.S. sites outside NASA and NCAR where a researcher could access a supercomputer. "That didn't seem strange to me, then," he recalls, so he went to work during the summer at the Lawrence Livermore National Laboratory.

Then in the summer of 1981 he was invited to the Max-Planck Institute for Physics and Astrophysics in Munich, where a Cray-1 supercomputer was available in an open environment. Smarr began a collaboration there with Karl-Heinz Winkler (now NCSA deputy director for Science, Technology, and Education) and with Mike Norman, whom Smarr had first worked with at Livermore. The Munich collaboration stretched over three summers and resulted in breakthroughs in the dynamics of extragalactic gas jets as well as plans for how a university-based supercomputing center should be organized. According to Norman, now NCSA research scientist and UIUC adjunct professor of astronomy, "Our jet research was launched on that Cray-1 in 1981. Every summer until '84 was spent doing research on the jets and brainstorming how to establish a supercomputer at the U of I."

"My eyes were really opened," Smarr says, "when Karl-Heinz asked why it was that so many American researchers had to come to Europe to work on U.S.-built supercomputers. Then he told me I should work to get a Cray X-MP at UIUC. I had never heard of the X-MP. He invited the Cray sales rep to speak at a conference we were organizing, and I got my hands on a color brochure. It really made me angry that not only did I have to go to Germany to use an American supercomputer, I had to hear about the new ones there, as well."



Larry Smarr in the summer of 1982 with an early version of a scientific visualization showing the evolution of a supersonic jet. While Smarr was at the Max-Planck Institute, the image was generated as a contour plot on a Cal-Comp plotter.

In the fall of 1982 when Smarr returned, he completed a paper that had its beginnings in sessions with Norman and Winkler. Norman recalls, "Larry sent copies of 'The Supercomputer Famine in American Universities' everywhere—it was really an underground protest, a call in the wilderness." Included in it were letters from dozens of researchers stating how their work was hampered by lack of computing power. One scientist estimated that calculations that would take him six years with his current equipment could be accomplished in two months of supercomputer usage. The overwhelming message was that research in the U.S. was falling behind the international competition.

The timing of this paper was propitious. In June of 1982 NSF had cosponsored a workshop on large-scale computing for a multi-agency panel headed by Peter Lax. The Lax Report appeared in December 1982. The following year, two NSF division directors prepared the Bardon-Curtis Report, essentially a blueprint for how NSF could meet the increasingly desperate pleas for supercomputer access. Smarr was an advisor on both of those reports, as well as the earlier Press Report, in 1981.

In 1983, after another summer of research and brainstorming in Germany, Smarr returned and in collaboration with other UIUC scientists and with George Badger, director of the Computing Services Office (CSO), wrote a proposal to NSF requesting a supercomputer for the campus. Recalls Winkler, "It was all there in that early proposal—some elements that still haven't been fully accomplished—visualization, the workstations, high-speed I/O, data storage, software development, and the close collaboration between users and the people running the place."

Unofficially, reports came back that the proposal stood a good chance of being funded. However, the bad news was that the new NSF program policy required a national competition to be held. Disappointed at the prospect of yet more delays, Smarr used the time to broaden its scope. Ted Brown, then UIUC vice-chancellor (now director of the Beckman Institute), proposed the title 'Center for Supercomputing Applications.' Smarr added the all-important adjective 'National.'

Once NCSA received funding in February 1985, CSO provided technical expertise and began negotiating equipment acquisitions, including the Cray X-MP/24 which was installed that August. Shortly before the Cray was delivered, Bottum flew out from NSF for a site visit. He was disconcerted to find that "Larry was already looking ahead to visualization and software, while back in Washington they were still wondering if anyone was really going to use those $20 million machines. He gave me a tour of the Water Survey Building before it had been remodeled, showed me where the training room would be, the conference rooms. There were drums of copper wire, light bulbs hanging from the ceilings. I thought, 'I just hope these people can get the *Cray* up and running. I hope they can get this thing *off the ground*.' Larry was talking about Macintoshes—*Macintoshes!* He was talking about $5,000 personal computers and we (NSF) had a $20 million investment here. He said Macs should be the windows into the Cray, but back then, when you used the word 'PC' in the same sentence as 'supercomputer,' people laughed. It was pretty nerve-wracking, that first visit."

Bottum returned to NCSA the next fall on a sabbatical leave, with two specific goals: to strengthen the national focus (which he did by establishing an outreach training program and the Academic Affiliates program), and to enhance user relations. For that, Bottum and Joseph Hardin, now manager of the Software Tools Group, set up the first online user survey. Somehow, by the end of his sabbatical year, Bottum had decided to remain at NCSA. His explanation? "Larry's commitment to the national program."

Karl-Heinz Winkler's reasons for accepting the offer to lead NCSA's scientific and technological advance into the 1990s are more introspective. "Back in the early eighties when we brainstormed in Munich, we tried to synthesize all the good and bad aspects of the various labs in which we had worked. So for the first five years NCSA was based on existing models. But from this point on, there aren't any models. In this rapidly developing technological environment, *we* will have to define the paths. It's a fantastic intellectual and professional challenge."

Mike Norman's first recollections of Larry Smarr date back to when Smarr convinced him to temporarily set aside his dissertation to work on some exciting extragalactic calculations. "Larry was then, as now, full of new ideas and worlds to conquer," laughs Norman. "It was infectious."

The assembled NCSA staff—many of them relative newcomers—were exposed to some of the famous Smarr vision when he addressed them in November 1989. "Frankly, when I began to think about a center like NCSA, I never dreamed of anything like this—it's like science fiction. . . . NCSA has pioneered the notion of a scientific research team working with a professional group of computer scientists, artists, software designers and others—involving their different talents to explore scientific problems. . . Out here in the cornfields has arisen a center of national and international impact, poised to be a major player in a major transformation of human society. . . . The world will not survive as we know it without the help of computational science."

Somehow, when Larry Smarr talks, one cannot help but catch the fever. ▲

Note: Jarrett S. Cohen, public information specialist, also contributed to this article.

Milestones at NCSA

1989

- FMC joined Industrial Partners Program
- Mass storage system upgraded with an Amdahl 5860 processor
- Interdisciplinary Research Program established in BI
- Donation of 62 Mac IIxes by Apple Computer Inc.
- Silicon Graphics Inc. established Renaissance Experimental Laboratory with donation of 25 IRIS Super System personal workstations
- National Science Board extended NCSA Cooperative Agreement with NSF through FY95
- UNICOS migration completed on the CRAY X-MP/48 system
- 200th employee hired in August
- Kodak extended its Industrial Program agreement
- Connection Machine (Model CM-2) installed in BI
- Dow Chemical joined Industrial Program
- Terabyte transition on mass store
- Visualization Services and Development Group completed hardware upgrade
- Caterpillar joined Industrial Program

The early days at NCSA

by William Dwyer, Graduate Assistant Editor

An anniversary issue would not be complete without stories of the "good old days" back when NCSA was getting started. Several of the people who were among the first to work at NCSA have shared their recollections.

So much to do . . .

The earliest employees of NCSA did far more than their job descriptions called for, because they were the only ones around to do it. Mike Smith, associate director of Computer Operations and System Administration, recalls when the first supercomputing system arrived—the $12 million CRAY X-MP/24. Employees had to take turns as around-the-clock security guards for the computer at the Astronomy Building for the first couple of weeks.

Sandra Moy, director of Computing at the University of Washington–Seattle, said she stayed with the Cray the first night. As associate director for Cray Facilities and CSO liaison to NCSA, she was in charge of the Systems Support Group who "lived" in the same room with the Cray supercomputer for the first couple of months. She said her duties ranged "from associate director to floor mopper," recalling the time she cleaned the Machine Room before the press conference for the new supercomputer. Moy remembers that the systems people would often be seen washing the large windows at the entrance to the Machine Room. "We were all really proud" to be working here then, she added.

Judy Olson in User Administration remembers truckloads of supplies and equipment pulling up outside and needing to be unloaded. As the only clerical person on the staff at the time, she had the somewhat difficult task of getting people like the student programmers to help with the unloading. Her job included answering the telephone, entering data into the computer, handling supplies, distributing mail, and so on. "Now we have a dozen different people doing those things," she said.

Dave Thompson, student programmer for the Software Tools Group, remembers unloading a truckload of "one or two tons" of IBM software. He said his duties, in addition to all of the programming and hardware-related tasks, included taking out the trash.

Bob Haber, NCSA adjunct professor and UIUC associate professor of theoretical and applied mechanics, said those early days offered a little bit more hands-on experience than now. He often had his hands in the back of cabinets of the visualization hardware—an experience Haber compares with working on the family car when in high school.

So little time . . .

In those early days, the work was never done. The same is true today, of course, but it was even more so back then. Larry Smarr's assistant, Jan Wehmer, said they worked 18-hour days for many months. She recalls her concern the time someone came into the office with a bad cold. "I was mad because she might give it to us," Wehmer said, because she felt they were too busy to get sick.

"I probably spent more time here than I did in my apartment," Mike Krogh, graphic applications staff member, remembers. At that time, he was a part-time student consultant and a junior in computer science trying to finish his degree so he could work full time at the center.

Design lead for the Software Tools Group, Tim Krauskopf, started to work for NCSA in January 1986, just before the center's grand opening at the Krannert Center for the Performing Arts. As a member of the then Workstation Development Group, he recalls scrambling to help put together demonstrations of the software for the grand opening. Ed Kubaitis, then manager of CSO Network File Systems and now senior research programmer with CSO, also remembers the activity and crises leading up to the opening. "It was kind of a big deal—a date cast in concrete" Kubaitis recollects.

Installing the CRAY X-MP/24 system. (UIUC News Bureau)

Kubaitis and Ross Veach, who recently rejoined CSO, were working on getting CFS up for the opening. "We got CFS ready a week ahead of target" and "a week before the Cray was up," Kubaitis recalls. After completing their work on a Saturday, they left a note on Sue Greenberg's door documenting the event. (Greenberg was an associate director of CSO, as now, and was responsible for NCSA's networking and CFS.) When Kubaitis and Veach arrived at work the following Monday, they found a balloon bouquet from Greenberg in appreciation.

Greenberg most remembers "the really great people who were unbelievably helpful" at sites that already had Cray systems. Part of her job was to travel to Los Alamos National Laboratory and Lawrence Livermore National Laboratory, where Cray systems were already in use, and to meet with people at the other NSF centers and with representatives from CRI. For her, it was "a very nice experience—the most memorable of all."

Donna Cox, NCSA associate director for Education and UIUC assistant professor of art and design, recalls that many of the early videos were produced as all nighters with "drop deadline" dates to meet. There was so much visualization work to do in the early days that Cox remembers

George Badger (then and now director of CSO) (left) and Ralph Simmons (then chairman of the Department of Physics and now a professor of physics) inspect the Cray system at the opening reception. (UIUC News Bureau)

"NCSA was the only place on campus where you couldn't find a parking space in the lot on weekends. Everyone was working all weekend long, just like another weekday—one crisis after another, one fire after another. Things really haven't changed," she adds, "only now we just have two parking lots and more people putting out fires."

And so little space.

Five years ago, the first NCSA people to take up residence in the Water Resources Building occupied three rooms on the first floor, a small space in the building that would gradually be taken over and renamed the Computing Applications Building (CAB). Space was at a premium and the mood was informal.

"You could hold a staff meeting in a very small room with the entire staff," Patricia Wenzel, manager of User Administration, said. The small space had its advantages and disadvantages. Wenzel said you could stand in the hall and, within a short time, meet and talk with everyone who worked there.

Charlie Catlett, now manager of Networking, recalls a staff pizza party that was held in a very small classroom of the Astronomy Building about a week after he came on board in November of 1985. The entire staff attended. Catlett noticed an older, gray-haired and bearded professorial-looking man in the room. "I just assumed he was Larry Smarr" since he was distinguished-looking, he remembers. "I hadn't met Larry yet." Catlett was surprised to discover that the "young guy with a beard" who later joined the party and inspired them with a talk was Smarr. And he was impressed with the fact that management threw a party for the staff.

Since space was tight, Jan Wehmer remembers calls coming in on one telephone that had a long cord. She would pick up the telephone and plop it on the desk of the person being called. And Brand Fortner, staff associate, had three or four computers on his regular-sized desk. "I had to stack monitors three high," he said, because he had four keyboards and three mouses taking up much of his desktop.

Fortner also remembers the pair of cockatoos someone had in the office that bit through the AppleTalk and Ethernet cables. There were frequent

Early days *continued on page 8*

Staff List
December 1985

Larry Smarr, Director
Win Bernhard*
James Bozek*
James Brennan*
Elizabeth Cardman*
Alan Carpenter*
Charles Catlett*
James Chiang*
Steven Christensen
Aaron Contorer
Karolyn Eisenstein
Cynthia Ejankowski*
Joan Flanagan
Nora Foreman
Brand Fortner
Suzanne Greenberg*
Katie Henry
Virginia Hudak-David
Mark Johnson
Ronnie Johnston
Ed Kubaitis*
Margaret Kubaitis*
Lex Lane
Lee Linton*
Thomas Madej*
Judy Melton*
Barbara Mihalas
Sandra Moy*
S. Natarajan
Judy Olson
Gaige Paulsen
Stanley Rankin*
Pamela Salela*
Renee Sawicki
Michael Smith*
Xiaohui Song
Jeffry Spengler*
William Taylor*
David Thompson
R. Ross Veach*
Harriett Weatherford
Jan Wehmer
Patricia Wenzel
Larry White
Edith Wickliff*
Bob Wilhelmson
Robert Wilson*
Alexander Wong
Shirley Yagoda*
Mary Young*

*Indicates CSO employee

Early days continued from page 7

jokes and not-so-amusing references to "roast cockatoos," according to Fortner, because "we were tired of cleaning their cages."

Dave Thompson came on board with three other undergraduates. By that time, NCSA had expanded to the second floor of CAB, and the four students shared a room with two desks in it—and one Macintosh computer.

Moves were frequent as the remodeling progressed. Bob Haber said he had to move six or seven times during the first year; he remembers the constant threat to expensive equipment from the dust of remodeling. Tim Krauskopf recollects moving from the second floor down to the first floor, then back up to the second floor, when the second floor was remodeled in the summer of 1986.

Today NCSA has grown to 240 staff members who occupy parts of five buildings (Beckman Institute, Computing Applications Building, Astronomy Building, Professional Arts Building, and the Oil Chemistry Building).

It was innovative . . .

Then, as now, the center's new technology presented unique challenges and prompted curious commentary. As Donna Cox reminisced, she recounted how she met Smarr and how one of her art colleagues reacted to her association with the center.

In the fall of 1985, Smarr visited the then-new computer laboratory at UIUC's College of Art and Design. Smarr met Cox who was working on a color project that eventually became ICARE (Interactive Computer Assisted RGB Editor). When Smarr issued an invitation to the Art and Design faculty to visit NCSA, Cox accepted. After becoming involved with NCSA, she participated in demonstrations at the NCSA Open House during the February 1986 grand opening. One person from art warned Cox that she was making a big mistake to work with NCSA. "It's bad enough that you do computer art," he said, "but now you're going to hang out with those scientists."

Scott Lathrop, associate director of the Academic Program, said it was difficult in the early days to convince someone from outside the area to come to NCSA ("Is that near Chicago?" people would ask), but not after the center gained national recognition.

Bob Haber said there was soon quite a bit of national attention focused on a small group of people. "That kept us hopping," he said. Haber also recalls the national concern about people from certain foreign countries gaining access to the supercomputer, which lead to a rather elaborate security system. He said "cloak and dagger" aspects of that time reminded him of James Bond films.

Some other ways of thinking have changed since those early days. For example, Harriett Weatherford, UIUC associate vice chancellor for research, said there were people at NCSA who didn't think they would need secretaries—because they had computers. (Until recently Weatherford was associate director of Finance and Administration at NCSA.)

Patricia Wenzel said Smarr wanted to have a "paperless office" back then. "I look at my office today and wonder what happened," she said.

Weatherford was teased by a fellow employee that she shouldn't take her pencil into a meeting with Smarr, or he might break it because it wasn't computerized. She said she also had to get up the nerve around that time to request a calculator, one that prints on paper tape, to put next to her computer.

Meetings in those days were considered "doing tea." Virginia Hudak-David, assistant director for Administrative Affairs, said Smarr had spent some time in England, so the staff met every Monday at 4 p.m. for tea and cookies. They would discuss their work and Smarr would give inspiring talks.

And it was worth it.

People involved with the center from the beginning have a special outlook about it. "Working for Larry Smarr was the best thing that ever happened to me," Patricia King in UIUC Administrative Information Systems and Services said about working for the NCSA director. "He has that sort of charisma that gets you caught up in his ideas," King said. As a secretary for the Computing Services Office, she spent over six months typing up the proposal for funding NCSA.

Jan Wehmer worked with Smarr in the UIUC Department of Astronomy before the National Science Foundation funded NCSA. She remembers the difficulties in getting the grant, and then the struggle to establish the center's supercomputing operation. She said they wanted to be the best, the fastest, and to set everything up before anyone else. People were dedicated to their roles in developing the center. "We felt that this was something the country needed, that the country didn't have," Wehmer said.

Joan Flanagan, now a computer consultant for Computer Guidance Service in Chicago, says the dedication and desire to help others learned in the early days at NCSA influences her work philosophy today. She remembers many nights of working late to get out the proposal to NSF when she

***Early days** continued on page 16*

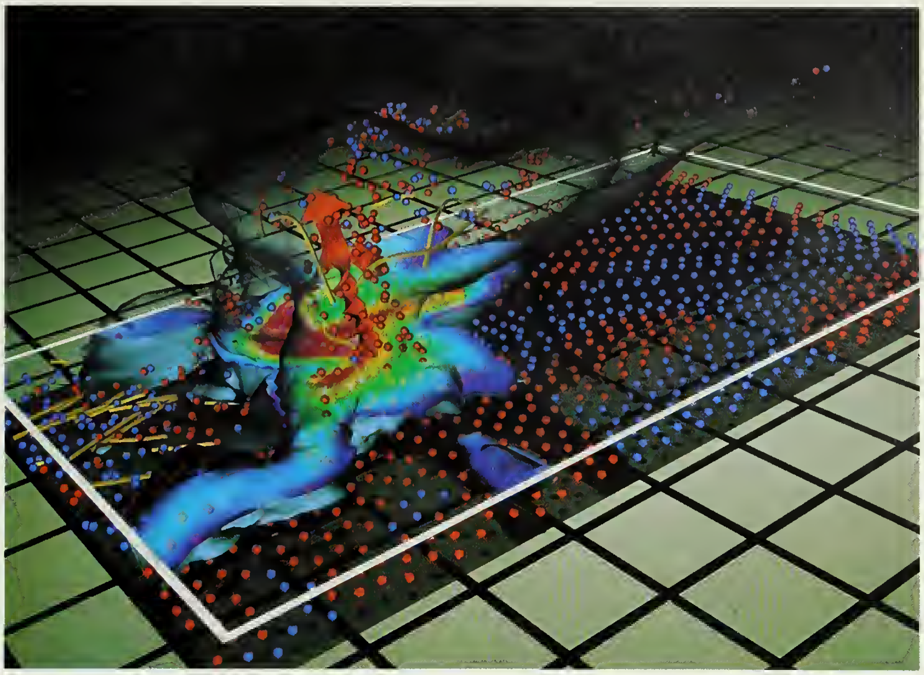
Training dates: 1990

February 12–16	New User Training
March 5–9	New User Training
March 26–30	Affiliates Training
April 23–27	New User Training

Note: Dates are subject to change. Class size is limited. You must register to attend NCSA training.
To register: Academic users contact Kendra Reasor at (217) 244-1100. Industrial partner users contact your representative at NCSA.
For additional information: Contact Lyle Rigdon at (217) 244-3659 or at lrigdon@ncsa.uiuc.edu (Internet) or 815@ncsavms (BITNET).

Tornado watch via supercomputers

by Randall Graham, Science Writer



Still frame from "Study of a Numerically Modeled Severe Storm." (NCSA visualization)

> *"I could see no sign of a tornado funnel this side of the greenish rain. But it was there, and my wife knew it was there. I told her to go in and take the children. . . . we had to take a chance on it missing us."* —Capt. Roy S. Hall, "Inside a Texas Tornado," *Weatherwise*, April 1987.

In the 23 years since Dr. Robert Wilhelmson, atmospheric research scientist at NCSA and UIUC professor of meteorology in the Department of Atmospheric Sciences, arrived at UIUC, tornadoes have killed nearly 2000 people according to *Storm Data* published by the National Oceanographic and Atmospheric Administration (NOAA). With the aid of supercomputer simulations, Wilhelmson wants to learn how tornadoes form. He envisions a day when forecasters will use simulations in real time, together with radar and other observations, to improve warnings and save lives.

"Within the next year, I am hopeful that our storm research group will, for the first time, successfully complete a thunderstorm simulation in which a tornado forms, " said Wilhelmson with excitement. "It will arise spontaneously from the data." When it does, it will mark a significant milestone in Wilhelmson's 20 years of storm research, because a tornado born from numeric data in a computer model can be analyzed to see how it forms and changes over its lifetime.

Wilhelmson came to UIUC in 1966 with a B.S. in Mathematics from Wheaton College to pursue a doctorate in computer science. He began writing software for the ILLIAC IV, a parallel computer then being designed at UIUC. But, said Wilhelmson, "I got tired of building stuff for compilers and I decided I wanted to use big computers to solve some type of physical problem." At that time, the university was launching a laboratory in atmospheric sciences headed by Dr. Yoshi Ogura (now retired). As a result of conversations with Ogura, Wilhelmson began to work on thunderstorm research, using his understanding of computers and numerical methods.

Constructing thunderstorm models

A thunderstorm model is a set of mathematical equations that describe atmospheric variables such as temperature, pressure, wind speed and direction, and moisture, water, and ice content. Wilhelmson solves such a model by dividing the atmosphere into small cubes in which these variables are updated every few seconds with the aid of a powerful computer. The result is billions of numbers that can describe the growth of small cumulus into large storms.

Thunderstorms and computing

The first large computer Wilhelmson used in the early seventies was an IBM 360/91 at the University of California at Los Angeles (UCLA). Remote access was available to this computer from UIUC over ARPANET, a national network initiated by the Advanced Research Projects Agency (ARPA) of the Department of Defense. "My Ph.D. came out of working with the IBM. It was the beginning of simulating thunderstorms using three-dimensional models," Wilhelmson recalls and then smiles. "We were simulating them in two dimensions before that. In that context it was possible to learn about the basic physics of the system, but it wasn't realistic for simulating real storms since they are three-dimensional in character."

In the mid-seventies he switched to a Control Data Corp. 7600 at the National Center for Atmospheric Research (NCAR) in Boulder, CO. "Initially I had to travel to Boulder to do my computing," remembers Wilhelmson. "ARPANET access to UCLA gave me an early look at the power and importance of networking. Without remote access, supercomputing had to wait until I could travel."

Travel to Boulder led to collaboration with Dr. Joseph Klemp at NCAR and Dr. Peter Ray, then at the National Severe Storms Laboratory in Norman, OK. This collaboration developed into important advances in understanding storm evolution through both modeling and observation in the late 1970s.

***Tornado** continued on page 10*

Tornado *continued from page 9*

In their research, Wilhelmson and his collaborators faced the problem of looking at the huge amounts of data generated on the supercomputer. In 1980, Wilhelmson met Larry Smarr (then an assistant professor of physics and astronomy and research astrophysicist, now full professor and director of NCSA). Both had the same problem and together built a visualization system called the VAX and Image Processing System with funding from their departments, the campus, NSF, and Arnold Beckman. They were later joined by Bob Haber (now NCSA adjunct professor and UIUC associate professor of theoretical and applied mechanics). With this system, Wilhelmson could use software developed at NCAR by Klemp for interactively looking at storm model output and could create two-dimensional animations of storm evolution.

Collaborating to establish a supercomputing facility

In 1983 Smarr and Wilhelmson joined several other researchers and UIUC Computing Services Office (CSO) staff to pursue a more ambitious goal—establishing a supercomputing facility at UIUC. Smarr had conducted a survey of over 65 UIUC professors and discovered that many were blocked in their research because they lacked supercomputer time. Those with time had to battle the inconvenience of accessing supercomputers at distant sites. But Smarr and other researchers wanted more than just a computer, they wanted a complete computing environment that would include systems to analyze the data generated. Wilhelmson recalls, "We thought in terms of a complete environment for solving computational problems that included hardware, software, and a collection of researchers, computer scientists, and staff that would work together to provide an interactive computer facility where 'breakthrough' science and engineering could be accomplished."

The group spent all of 1983 drafting a proposal to the National Science Foundation with considerable input from Michael Norman, now NCSA research scientist and UIUC associate professor of astronomy, and Karl-Heinz Winkler, now NCSA deputy director of science, technology, and education, who were both in Munich, Germany at the time. By February of 1985, NCSA became a reality. "There were only a few of us on board in the beginning, outside of the CSO staff who were responsible for facilities management," remembers Wilhelmson.

Bob Wihelmson.

As assistant and associate director at NCSA for several years, Wilhelmson helped guide the growth of NCSA. His storm research group now spends

Tornado *continued on page 16*

1988-89 *Science Nuggets*

Thanks to the following scientists who cooperated with Paulette Sancken, publications editor in the Information and Publications Group, to produce a list of science nuggets that was submitted to NSF in December 1989:

Beverly K. Berger
Oakland University, Physics
Numerical Simulations for Quantum Cosmology

Ernest R. Davidson
Indiana University, Chemistry
Quantum Theory of Molecules

Robert C. Frank
Augustana College, Materials Research
Trapping of Small Atom Impurities by Lattice Defects in Metals

Karl Hess
UIUC, Electrical & Computer Engineering
Monte Carlo Simulation of Femtosecond Spectroscopy in Semiconductors

Morris Huck, UIUC, Agronomy
Robert Grant, University of Alberta, Agronomy
Simulation of the Elementary Processes Involved in Crop Growth

Richard Matzner
University of Texas, Astrophysics
Numerical Studies of Inflation in Backreacting Cosmologies

James McCammon
University of Texas, Chemistry, Molecular Bioscience
Theory of Biomolecular Structure and Dynamics

Ahmed Noor
George Washington University & NASA Langley, Materials Engineering
Finite Element Analysis on Multiprocessor Computers

Klaus Schulten
UIUC, Physics, Molecular Bioscience
Molecular Dynamics Simulations of the Photosynthetic Reaction Center of Rhodopseudomonas viridis

Almon G. Turner
University of Detroit, Chemistry
The Role of X-NO_2 Type Molecules in Ozone Depletion Cycles

Robert Wilhelmson
NCSA & UIUC, Atmospheric Sciences
Understanding Storm Model Simulations through Visualization

NCSA's Industrial Program

by William Dwyer, Graduate Assistant Editor

Caterpillar recently became the seventh full partner to join NCSA's Industrial Program and the third corporation to do so in 1989. FMC Corporation and Dow Chemical joined earlier last year. The newest partner signed a three-year, $3 million agreement in December. Since 1986, when Eastman Kodak joined, industrial partners have invested over $25 million in NCSA through their corporate agreements.

The Industrial Program is the major force in NCSA's mission "to strengthen the industrial competitiveness of American industry" using the tools and techniques of leading-edge computational science. The head of the program, Associate Director John Stevenson, plays a significant role in making that happen. He developed the marketing plan for NCSA—the "product"—which he defines as "a package we offer corporations to solve their problems."

Industrial partners

Eastman Kodak Company
Joined NCSA in August 1986
Extended in June 1989

Amoco Corporation
Joined in July 1987

Eli Lilly and Company
Joined in November 1987

Motorola Inc.
Joined in December 1987

FMC Corporation
Joined in February 1989

Dow Chemical Company
Joined in October 1989

Caterpillar Inc.
Joined in December 1989

In November 1985 Stevenson was loaned to NCSA to develop a marketing strategy that would satisfy NSF grant requirements. His high-level corporate expertise—he was an officer at AT&T in charge of marketing—was used to put together a marketing plan for an industrial program and to implement it in time for the grand opening of NCSA in February 1986. Within that short period, he helped develop a strategy that included an advertisement in the *Wall Street Journal* and a letter and brochure to each of the "Fortune 500" corporations' CEOs.

Defining the benefits

Stevenson says that corporations are getting much more than time on a supercomputer when they join NCSA's Industrial Program. They are getting a package that contains about 14 categories of support including training on the supercomputing systems, use of the visualization resources, software, and use of state-of-the-art hardware. The support package comes with a full partnership agreement—a three-year minimum contract that a corporation negotiates with NCSA.

"It takes at least a year to a year and a half of meetings and negotiations to sell the program," Stevenson says about the complex interaction with prospective industrial partners. All agreements are tailormade to suit each corporation's needs. Since the program's inception, over one hundred corporations have visited NCSA. With over 250 additional high-level executive visits, the industrial exposure of NCSA has been enormous.

A new offering of the Industrial Program is an associate partnership—a one-year agreement that includes a week of extensive training and consulting support during the year. It is an entry-level program for corporations with little exposure to supercomputing and computational science.

John Stevenson.

Stevenson divides his time between managing the accounts, which means providing the necessary support to current partners, and marketing, the continuing process of informing corporations about the program. Two assistant directors, Jeff Simon and John Patten, help supervise the management of current contracts [see ***access***, November–December 1989].

To market NCSA, Stevenson says he employs the "5 P's." They stand for product management, promotion, price, place (or distribution), and the one he says is the most important, people. "None of this happens unless you have people." And one of the best reasons for developing a supercomputing center was to bring together academic and industrial people, he says. Over the years in America, the two researching groups have grown apart in the real world, but NCSA is trying to bring them back together and, he adds, "We've been very successful promoting the interaction."

Meeting the national challenge

Getting the various groups to work together is part of a national effort to support U.S. economic competitiveness and productivity, one of the goals of the President's Office of Science and Technology Policy (OSTP). The OSTP's Federal High-Performance Computing Program plan calls for a federally

Industrial *continued on page 12*

Industrial *continued from page 12*

coordinated government, industry, and university collaboration.

Responding to the partners

Eastman Kodak, NCSA's first full partner, joined the program in August 1986. Kodak also became the first corporation to extend its original agreement in June 1989. Stevenson says that Kodak and the other full partners recognized the importance of being out front, and the NCSA Industrial Program is one way they can stay there. Eli Lilly and Company, who brought their board of directors to NCSA in 1988, are in the process of getting their own Cray system to expand supercomputing research started at NCSA.

In August 1989, Lilly produced a research application workshop, "FOCUS on Chemistry Using Supercomputers" [see ***access***, November–December 1989]. Stevenson says the workshop was designed by Lilly using NCSA's facilities to stimulate new users within their corporation. The response was so great that Lilly plans to produce several more workshops.

FMC Corporation, which became a full partner in February 1989, independently produced a video showing their use of NCSA supercomputer systems and visualization software. The video exemplifies how the Industrial Program works, and how it can be applied successfully to the needs of an industrial partner. It also dramatically illustrates the application of NCSA's scientific visualization software.

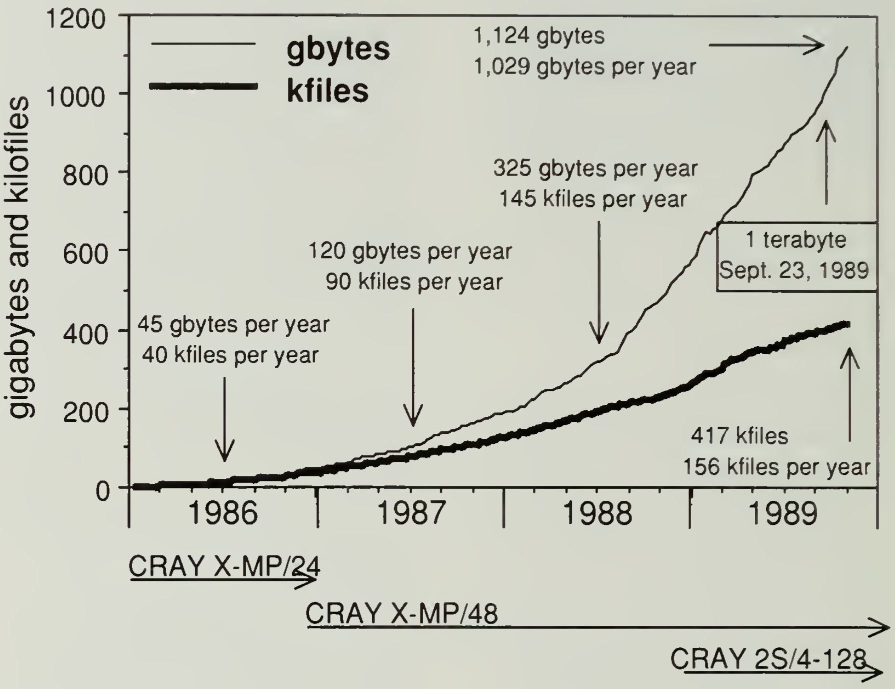
Motorola has also produced a video showing electric fields around the components on a circuit board [see ***access***, July–August 1989]. Motorola has been working with NCSA's Software Tools Group and Scientific Media Services to increase the efficiency of generating video animations from their simulations.

Dow Chemical has put 18 people through NCSA's new user training program since it joined in October 1989. Dow plans to devote a significant amount of its effort toward chemical engineering applications requiring computational fluid dynamics. James Rieke, Dow site manager,

Industrial *continued on page 16*

NCSA terabyte transition

by Curt Canada, Systems Programmer



CFS storage.

Fast reliable access to files is essential for effective use of a high-performance computer. The NCSA mass storage system (MSS) achieves this through use of the network-based hierarchical Common File System (CFS) software developed at Los Alamos National Laboratory (LANL) and enhanced at NCSA. CFS and its companion MASS/CFS utilities on the CRAY X-MP, CRAY-2, and VAX front-ends provide NCSA researchers with access to highly reliable and cost effective storage devices for long-term file storage.

The growth history of CFS storage has been dramatic (see graph) and has recently passed a significant milestone. On September 23, 1989 (the author's birthday) at 1:09 a.m., the trillionth byte was stored into CFS. This "terabyte transition" occurred near the beginning of a 33,517,568-byte save request from the CRAY X-MP by Jian Shen of the University of Houston.

This event occurs at a time when NCSA is about to embark on several projects to improve users' access to and ability to interpret their data. These projects range from a high-performance UNIX-based replacement for CFS to an ultra-high-performance disk farm to intelligent user interface data management tools. ▲

Visualization wins again and again

by Fran Bond, Technical Editor

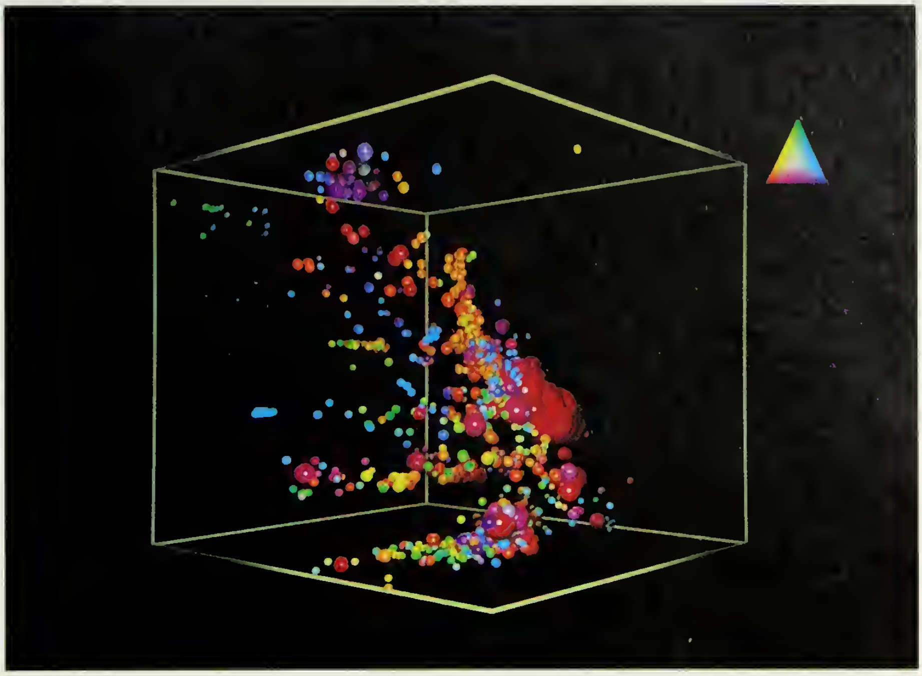
"Study of a Numerically Modeled Severe Storm," a recent NCSA-produced videotape, won the Visualization Award (representing first place in the Visualization category) at the Computer Graphics Film Festival 1989 held in London, England in November 1989. Known as "Europe's premier showcase for the latest computer graphics technology and applications," the film festival was in conjunction with the Computer Graphics '89 Conference.

Recently the videotape was accepted for viewing at the International Festival of Cartoons and Animated Films, February 23–March 4, 1990, in Brussels, Belgium. Produced in July 1989, it was chosen for showing at ACM's SIGGRAPH '89 Conference, Boston, MA in the film and video show, August 1989 [see ***access***, September–October 1989]. The videotape was one of the best 44 out of 328 entries submitted for viewing.

Those who worked on the award winner are Robert Wilhelmson, Harold Brooks, Brian Jewett, Crystal Shaw, and Louis Wicker (Scientific Research); Matthew Arrott, Mark Bajuk, Colleen Bushell, and Jeffery Yost (Scientific Visualization); Dan Brady, Randy Butler, Kathy Robinson, and Roger Francisco (Production Support); and Vincent Jurgens, Bob Patterson, and Cordelia Baron (Post Production). (See page 9 for a still frame from the videotape.)

Previous awards

NCSA's pioneering visualization effort has won recognition around the world. The Advanced Visualization Facility for Computational Sciences was first designed in fall 1986. By July 1987 the earliest entry for competition had been completed. A list of outstanding visualizations follows:



Still frame from "Scientific Visualization '88." (NCSA visualization)

"SCIENTIFIC VISUALIZATION '88" (produced July 1988)—accepted for film and video show, ACM SIGGRAPH Conference, Atlanta, GA, August 1988; award in Computer Graphics category, The Film Festival, London, England, October 1988; Grand Prize and Silver Prize in Scientific Computer Graphics category (500,000 yen or $3, 879.31), AV Software International, Nicograph Conference, Tokyo, Japan, November 1988; accepted for showing in Pixel-INA Awards Competition, Imagina '89, Monte Carlo, February 1989; Grand Prix in Visualization category, Parigraph '89, Paris, France, March 1989; Second Place in Scientific Visualization category, National Computer Graphics Association Conference, Philadelphia, PA, April 1989; accepted for showing at Pavilion of the World Design Exposition (50,000 yen or $390.00), World Design Exposition '89, Nagoya, Japan, July–November 1989; Silicon Graphics Award for Scientific Visualization (3,000 francs or $1,844.00), Computer Animation '89, University of Geneva, Switzerland, June 1989; accepted for showing in the Electronic Theater, Graphics Interface, London, Canada, June 1989.

"PROJECT SCI-VI" (completed July 1987)—Special Award in Computer Graphics category (monetary award also), AV Software International, Nicograph Conference, Tokyo, Japan, October 1987; Second Place in Science and Industry, Computer Graphics category, National Computer Graphics Association Conference, Anaheim, CA, March 1988.

Other honors include an Award of Excellence for *Science Highlights '88* awarded by the Society of Technical Communication, Chicago chapter, in its 17th Annual Technical Publications/Art Competition, December 1989. The brochure's cover featured a collage of stills from a variety of visualizations produced at the center. Colleen Bushell and Stefen Fangmeier were art director/illustrator and technical director respectively for the artwork.

In April 1988, NCSA's 1987 Christmas card, illustrated with visualization stills, won First Place in the Illustration category for the annual CHAAMP award competition of the Ad Club of Champaign-Urbana.

Formerly called Scientific Visualization and Media Services Group, the group is now Visualization Services and Development. Dan Brady continues as the group's manager (see **NCSA Contacts**, page 15). ▲

NCSA software

by Joseph Hardin, Manager, Software Tools Group

When the Workstation Development Group (WDG) was established in the fall of 1985, its focus was largely directed inward. The workstation (then, a Sun, Mac Plus, or IBM AT) was to be a "window to the Cray" for users, and a lot of time was spent developing local networks, utilities, and facilities at NCSA. But one real development project was taken on: providing remote users with Mac and IBM access to the center across the fledgling NSFNET. Early in 1987, WDG released NCSA Telnet into the public domain. For users and the group, things would never be the same again. NCSA software was entering the national scene, and a new model of software development that met the needs of computational science emerged.

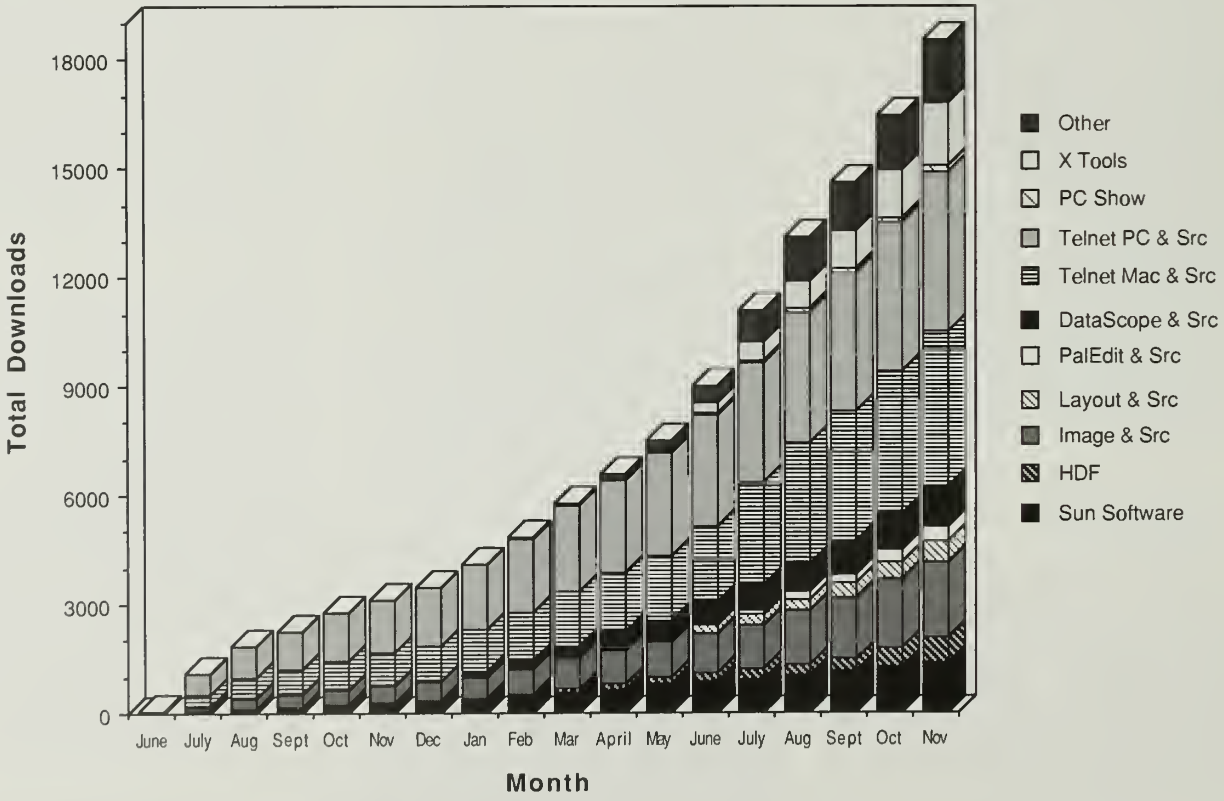
That same year, a research scientist/graduate student team at NCSA put together a Sun program for color raster images. WDG documented this version and developed another version for the new (color capable) Macintosh II. Thus, NCSA ImageTool was released in late 1987.

The next fall, NCSA DataScope for the Mac was released by the newly dubbed Software Development Group (SDG). The needs of a networked environment were demanding a data transport system that was transparent to the user, portable across machines, and had multi-object storage capabilities. In response to these needs, NCSA Hierarchical Data Format (HDF) was born, and its first release, in June of 1988, has been followed by continuous development.

SDG waited out the stormy X Windows vs. NeWS debates, and then, in the winter of 1989, started development of a group of X Window color raster and 3D color tools. This fall, NCSA X Image and NCSA X DataSlice were released and included on the MIT X11 release 4 distribution tape. The model worked again.

By this time the number of downloads from the newly named Software Tools Group's (STG) anonymous FTP server was over 1,000 packages a month. Adoption by the national user community was continuing to explode.

In the spring of 1989, a full suite of color raster data analysis and visualization tools for the Mac called the Scientific Visualization Software Suite was available officially. NCSA's model of quality, no-strings-attached, well-documented software developed in close cooperation with computational scientists was solidly established. ▲



Accumulated totals June 1988–November 1989. The number of users who are obtaining NCSA software and source code by download steadily increases. See the December 1989 *Technical Resources Catalog* for a list of available software.

NCSA Contacts

General information and machine access

NCSA Receptionist
(217) 244-0072
FAX (217) 244-1987

Orders for Documentation and Publications
Debbie Price
(217) 244-4130

Cray Operations
(217) 244-0710

Dialup Access—2400 baud or less
(217) 244-0662

Dialup Access—9600 baud
(217) 244-6733

CRAY X-MP IP address
ux.ncsa.uiuc.edu (128.174.10.46)

CRAY-2 IP address
u2.ncsa.uiuc.edu (128.174.10.44)

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ncsab.ncsa.uiuc.edu (128.174.5.101)

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***Industrial** continued from page 12*

says, "The Cray computers, the new Connection Machine, and the ability to visualize many of our process operations make NCSA an ideal location to gain new insights.

Stevenson says that scientific visualization has been a major development at NCSA, and, in terms of change since the early days at NCSA, it is "the biggest one, without question." He points out how useful visualization techniques are for company researchers who need to explain their ideas to management.

Helping solve problems

But Stevenson then immediately qualifies his statement by saying that the training aspect at NCSA is equally important. He also praises the Applications Group, headed by Associate Director Michael Welge, and the Industrial Consultants for their tremendous support to the corporations. These people provide each partner with expertise in how to use NCSA's hardware and software and in how to solve specific problems.

Stevenson says the work of Harrell Sellers and his people in the Computational Chemistry Group has been outstanding. With the help of this group, NCSA has played an influential role in moving the chemical industry into supercomputer applications.

The program's many achievements, highlighted by NCSA's teamwork and dedication, are major reasons NCSA has been so successful, Stevenson says. The accomplishments of the program's partners are reverberating throughout industry. As the word about successful Industrial Program partnerships gets around, other corporations will turn toward the use of advanced computing as well. This process makes our country more competitive, which is one of NCSA's primary goals. ▲

***Early days** continued from page 8*

was a student employee in the astronomy department. "Mostly Larry's enthusiasm" caught her up in the project, and the "tremendous effort working together as a team" with Smarr and Wehmer was like being in a family. "Larry's energy ignites enthusiasm with everyone to put out their best," she went on. To date, Flanagan says her favorite job is the one with NCSA because of the people and excitement.

Mike Smith said it was a very rewarding experience to have been involved from the beginning, and the people who were here at that time have a vested interest in the center. Smith said he doesn't miss the way it was in the early days at NCSA, because the challenges for him are still the same. "You're always trying to do something better for the users," he said. "That's what you're doing it all for anyway." ▲

***Tornado** continued from page 10*

time participating in development work and prototyping with other NCSA staff and utilizing the NCSA facility for storm research. He says that "It has been exciting for my group to work with other NCSA staff in the development and testing of new hardware and software tools for accessing and viewing the gigabytes of data that a single model simulation creates and, more generally, in contributing toward NCSA's goals."

Wilhelmson looks forward to continually sharing developments at NCSA with the community of atmospheric researchers. And he is excited about the center's environment. Said Wilhelmson, "NCSA has become a magnet that draws people together from disciplines that would otherwise never have contact with each other. It is breaking down artificial walls that have stood between us for so long. I'm glad to see that." ▲

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data link Contents

- GNU Emacs now available on the Cray systems
- NCAR Graphics update
- Engineering software update
- Making LOCAL improvements to CRAY-2 Fortran code

If you want to receive a copy of the current ***data link***, contact Debbie Price at (217) 244-4130

Subscriptions

Mail to Tammie Hildreth, Information and Publications, NCSA, ***access***,
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February 1990 vol. 4 no. 2

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Software

Software developed for molecular biologists

by Jill Peacock, Editorial Assistant, Software Tools Group

The NCSA Software Tools Group (STG) has just released a new visualization and analysis tool for molecular biologists. NCSA GelReader 1.0, released in mid-February 1990, is the first discipline-specific program from STG.

STG will create more discipline-specific tools while continuing to improve the generic data analysis tools in the NCSA Scientific Visualization Software Suite [see ***access,*** July–August 1989].

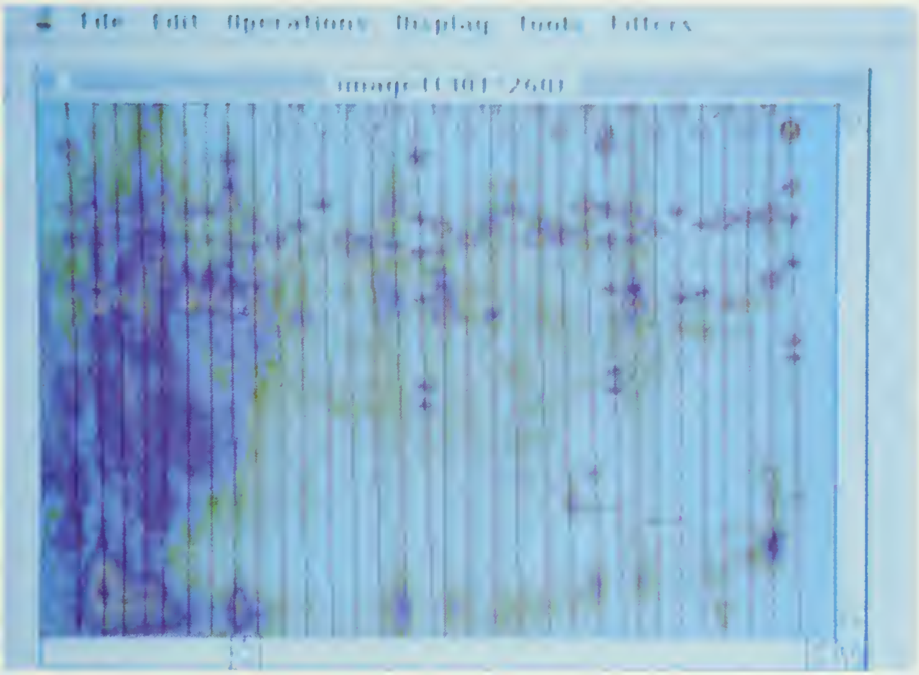
GelReader, developed by STG senior programmer Thomas Redman, has resulted from a combined effort with researchers at the Center for Prokaryotic Genome Analysis (CPGA) and UIUC Assistant Professor of Plant Biology Tom Jacobs. Redman says, "Without the professional critique and collaboration of CPGA and Tom Jacobs, the project would have stagnated." Redman further credits CPGA as "instrumental in initiating the GelReader project," adding that during the development of the program, "CPGA's comments and cooperative efforts were invaluable."

GelReader, then in a prerelease version known as Gene Mapper, was first introduced to the molecular biology community in August 1989 by Brand Fortner and Larry Smarr at MacroMolecules, Genes, and Computers: Chapter Two International Symposium and Workshop. Smarr, NCSA director, was a conference participant and Fortner, then manager of NCSA applications software, demonstrated Gene Mapper and other NCSA software for the Macintosh.

What GelReader does

GelReader helps scientists extract information from digitized electrophoretic gel images. Specifically designed for molecular biologists analyzing genomes, GelReader is also useful to anyone who needs to analyze electrophoretic gel data. The program

Software *continued on page 3*



Above. An example of NCSA GelReader analysis of electrophoretic gel data. GelReader's ether palette is demonstrated with the lanes and bands shown. The vertical lines represent the lanes while the horizontal dashes represent the bands.

Caterpillar is newest industrial partner

see page 7

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Abbreviations

CRI	Cray Research Inc.
IRC	Interdisciplinary Research Center of NCSA
NCSA	National Center for Supercomputing Applications
NSF	National Science Foundation
UIC	University of Illinois at Chicago
UIUC	University of Illinois at Urbana-Champaign

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***Software** continued from page 1*

uses the color-imaging capabilities of the Macintosh to help biologists estimate the sizes of eletrophoretically separated DNA fragments.

GelReader enables users to do the following:

- view a digitized image of the bands made by restriction enzyme digestion of DNA
- display the image in a variety of gray scales or color shades
- use histogram equalization to enhance image contrast
- use image shadowing to accentuate bands
- crop the image to the area of interest before analysis
- specify (or let the software determine) the number of lanes present in the image
- indicate the identified lanes with a user-selected color
- edit interactively the lanes in the image
- identify presumptive bands in each lane automatically
- adjust the sensitivity of the band-searching procedure
- view and edit the band identifications interactively
- identify lanes containing size standards and associate molecular weights (sizes) with the bands in those lanes
- generate reports of band locations or molecule sizes inferred from curves fit to the bands in the standard lanes

DNA fingerprinting with GelReader

Scientists, some located as far away as Australia and the United Kingdom, are now testing and using GelReader in their research. Steve Fletcher, working in the home office of Britain's Forensic Sciences Service, incorporates NCSA GelReader in his studies on DNA fingerprinting. This controversial process provides a unique way for scientists to identify an individual, not only by a fingerprint but also from any mammalian DNA source. Although DNA identification faces extensive judicial challenge, the technique may tremendously help—and in some cases already has—current methods of criminal investigation.

Genome analysis

Biologists' need for a tool such as GelReader is great. Eric Lander, a member of the Whitehead Institute and associate professor in the Department of Biology at MIT, is involved in a projected four-year effort to construct a map of the mouse genome. This map will help him compare many different DNA clones and detect which ones overlap each other. In Lander's words, "You have to quantitatively compare something like 20,000 images. That may be 40 lanes per image, or some 800,000 patterns." With such a large number of items to study, Lander and his coresearchers realized that they would have to either develop some type of analysis program themselves or search for an existing one. "We were pleased to find a program that had our problem essentially solved; we couldn't have proceeded otherwise," he says.

> *"My interest in this project has been and continues to be development of software for everyone; that is, for the molecular biologist in the modest laboratory."*

At UIUC both groups and individual researchers see uses for the GelReader tool. Members of the Center for Prokaryotic Genome Analysis (CPGA), headed by Carl Woese and Jordan Konisky [see ***access***, January–February 1989], are trying a novel approach to DNA analysis. Like Lander, CPGA researchers are mapping genomes. Pieces of DNA are first cut with restriction enzymes that reveal the patterns of each DNA sequence. The patterns are studied and overlapping ones are detected. Using this method scientists can map the location of pieces of DNA on an entire genome. Once that process is completed, they can start breaking down DNA pieces further and sequencing them.

Patrick Gillevet, UIUC research scientist in microbiology and member of CPGA, explains the ultimate conclusion of the research. "Once you have determined the DNA sequence, you know where the genes are. We do evolutionary studies with this information by looking at these genes and how they evolved. We can also determine how the genome is organized, and how it evolved." Gillevet says that GelReader "has helped in the analysis and saved us time in our work."

Traditionally, individual biologists have first studied a specific area or a specific gene of a DNA sequence and then combined the results into a cohesive whole. "They would work from the bottom up," says Gillevet. CPGA's approach, as well as one of the aims of GelReader, is to work from the top down. Gillevet says, "We're basically trying to sequence the whole genome at once. That's the new trend right now and also the rationale behind the Human Genome Project." The Human Genome Project was initiated in 1986 to find the sequence of genetic information on humans' 46 chromosomes in order to provide novel information on the origin and processes of life. In addition, the research may point to cures for genetic and organic diseases.

Individual analysis

When Tom Redman created GelReader, he had in mind that this tool as well as future NCSA discipline-specific tools "should be globally useful—if not across a number of sciences, then at least extensively across one science." In the area of biology, GelReader has certainly reached this goal. The research by both Lander and Gillevet uses the tool on large-scale DNA analysis by groups of researchers, whereas Tom Jacobs'

***Software** continued on page 18*

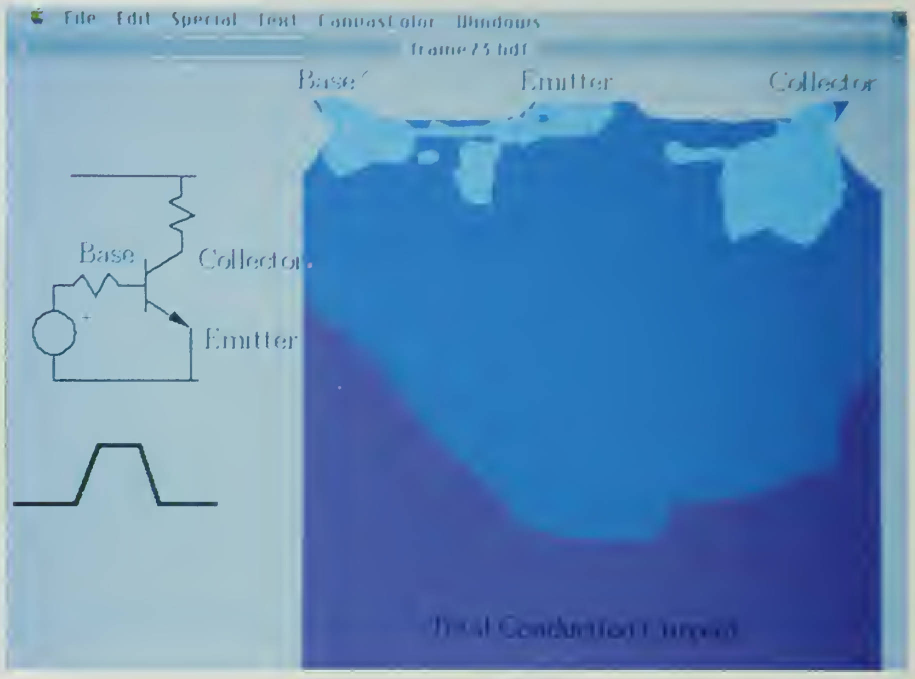
Expanding the uses of NCSA software

by Jill Peacock, Editorial Assistant, Software Tools Group

The impact on scientific research of the NCSA Scientific Visualization Software Suite [see ***access,*** July–August 1989] is becoming increasingly widespread as more users apply the tools to their own work. Dr. Arthur Raefsky, senior research associate for the Center for Integrated Systems headed by Robert Dutton at Stanford University, has used the suite not only in educational areas but also in his own research. He feels that software such as NCSA Image and the attitude of NCSA staff "have been of immeasurable help and made a fundamental difference" in both research and education.

Explaining the impact of NCSA tools on the educational side of his work Raefsky says, "I guess what's underway here is the whole effort to combine a lot of the simulation codes that we have with graphical interfaces and visualization—all built together in one program. And what we really want to do is use the resulting program in a number of our courses on the Macintosh to actually teach numerical simulation methods to both undergraduate and graduate students in electrical engineering. One of the major things we've been able to do is take parts of the NCSA Image software, combine them very closely with our simulation tools, and build a user-interface on top of both the simulation and visualization tools. In this way an electrical engineering student could really start to interact with the analysis codes we have. The fact that NCSA Image was distributed software in the public domain was just incredibly valuable to us. We didn't have to reinvent the wheel."

"In the last six months, I would say not a single graduate student has presented his thesis without showing a video using NCSA software tools."



Above. A single frame from a sequence created by electrical engineers at Stanford University using NCSA Layout. The sequence, of a bipolar transistor using the Stanford BiCMOS Process, enables students and researchers to observe total conduction current changes within the transistor.

Giving students experience

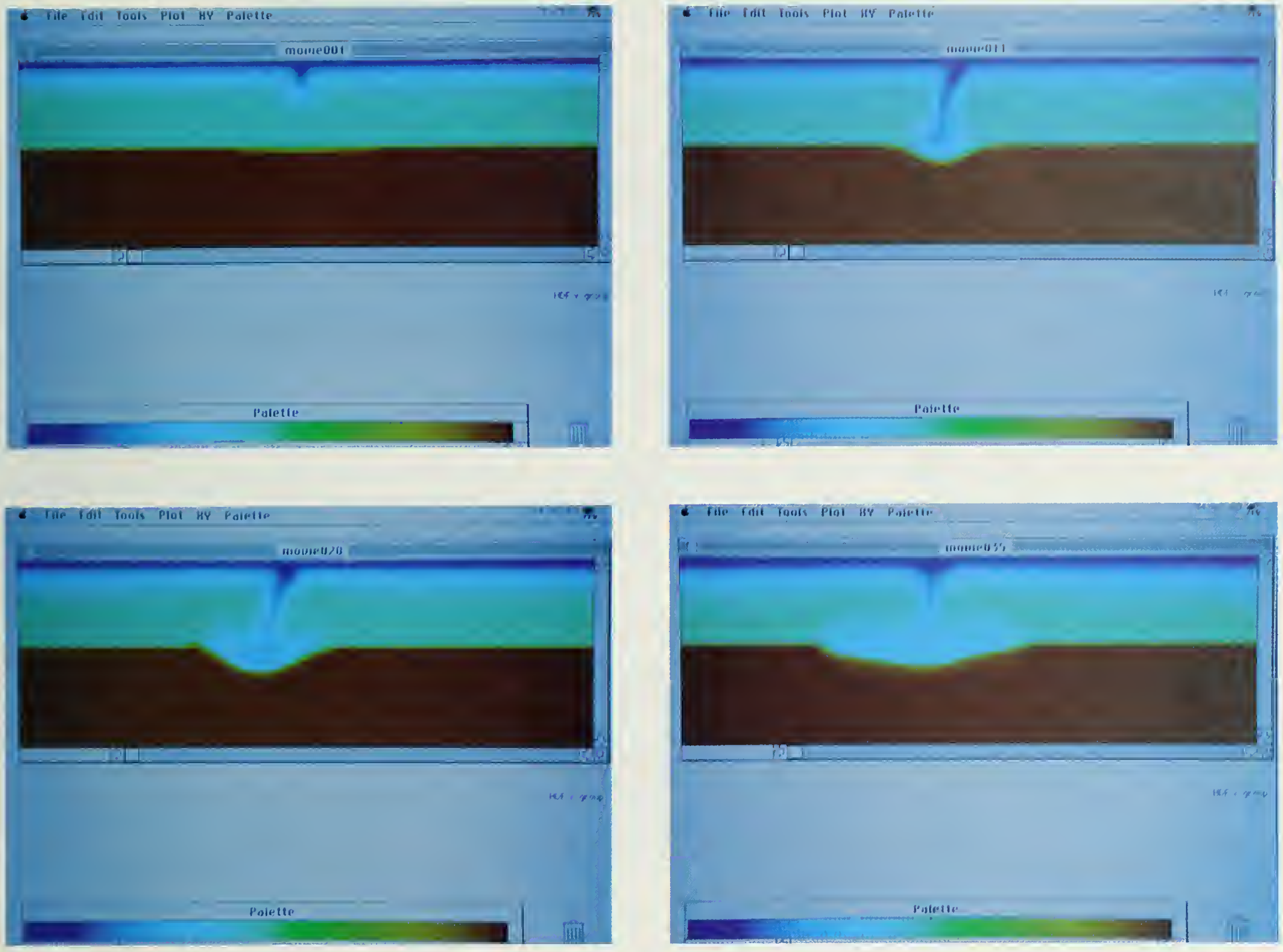
Before the NCSA tools were introduced, students could not gain practical experience in viewing and understanding visualizations of datasets. Therefore they were somewhat disadvantaged once they entered a real-world situation. Raefsky explains this dilemma: "With classroom experience, you generally learn very simple methods that don't apply in industry. As a result, a person really has to learn to use computer modeling techniques on the job. NCSA tools give us the ability to teach not only analytic but also simulation and numerical methods that in turn permit the student to understand all three and how they interact."

Raefsky goes on to explain how software tools from NCSA, *Mathematica* from Wolfram Research, and simulation codes from Stanford are integrated to increase students' understanding: "We've done some work with *Mathematica* in which we've been able to visualize mathematical solutions in very much the same way that some of the numerical modeling codes present their solutions. In this way students can learn to think physically in terms of what a graphic or visualization of some computer model means. For example, when you learn mathematical modeling, you learn to think about the meaning of differential equations and their answers in terms of the physics in some real, fundamental sense. Through using *Mathematica*, combining the NCSA Image program with our simulation codes, and building an interactive environment, we've been trying to teach the physical reality behind the numerical methods."

In addition to changing how students are taught, NCSA tools have altered the way students prepare their final presentations. Raefsky says, "In the last six months, I would say not a single graduate student has presented his thesis without showing a video using NCSA software tools."

Creating new software

Graduate students and research associates Peter Griffin, Goodwin Chin, Robert Huang, and Greg Anderson have been working with Raefsky on such programs and



Above. Sequence of NCSA Image screens showing convection problems of the earth's mantle. These are only 4 frames from an 80-frame animation created by Arthur Raefsky and Scott King using NCSA software. In this sequence the earth's crust is represented as a slab that is heated and reabsorbed back into the mantle. The colors represent temperature, with red being the hottest and blue the coolest.

combining them with a code called SEmiconductor Device ANalysis (SEDAN). SEDAN is similar to PISCES and SUPREM codes, which are interactive device modeling programs that are installed on the NCSA Cray supercomputers. Because PISCES and SUPREM are more advanced simulation tools, "they would easily overload the computational capabilities of the Macintosh."

Raefsky discusses accomplishments of his group in the area of electron device simulation: "What we've done is write a program using SEDAN that links the NCSA Image software to PISCES and SUPREM, but that is not as interactive as those two. Usually you go off and do your simulation run on the Cray. The device program then takes the results from the simulation program and brings it back to NCSA Image, where you see the visualization. What we're doing with SEDAN is teaching people to combine those steps.

"A lot of what we'll learn as the power of the Macintosh or the Sun really starts to increase is that we can incorporate those ideas in the advanced tools we'll be building. In fact, I think that because of our experience with combining the device simulation code directly with desktop visualization, the whole next generation of software we're developing at Stanford will have a lot of those capabilities built in from initial design.

"So SEDAN and NCSA tools are not only very valuable to what you learn in the classroom, but they also provide a good model for the future evolution of our software, especially given what the capabilities of desktop computers are going to be in two to three years. I really see Cray-like power on the desktop within two to three years."

Working interactively with software

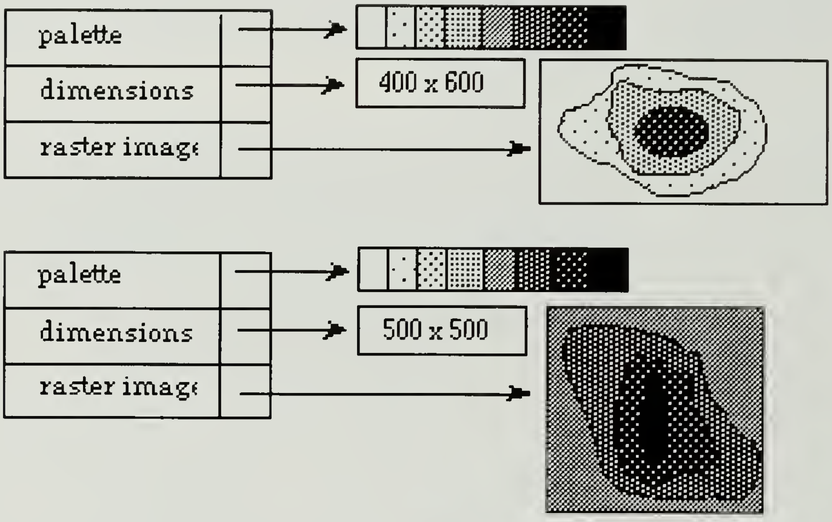
"The exciting thing for us is that we're really starting to understand how you combine interactive interfaces with visualization and simulation in a much more closely knit way, where the visualization is really giving you the progress of an algorithm," says Raefsky. "You're not just computing a solution, then viewing it. You're viewing it as it's being computed. In the phenomena we're doing now, which is highly nonlinear, by just watching the way the algorithm is performing and being able to interact with it, we often can use our physical knowledge to help along the progress of the algorithm—to help it do its job better than we could ever do with just plain mathematical techniques. Interaction won't be limited to

Expanding *continued on page 17*

Newest version of HDF released

by Michael Folk, Senior Programmer, Software Tools Group

HDF 3.0 has now been officially released after many delays. HDF 3.0 is supported on the Sun, Cray, Macintosh, SGI Alliant, and IBM PC machines at NCSA. Support for non-NCSA VAX/VMS systems is expected soon.



NCSA HDF is a standard file format for storing scientific images, data, and other information in a file. NCSA's tools and other visualization software read and write HDF files. This figure illustrates the storage of two 8-bit raster image sets in an HDF file. Each set consists of a color palette, the dimensions of the image, and the image itself. The HDF 8-bit raster image interface provides routines for storing and accessing raster image sets in HDF files.

All of the features of HDF 2.0 [see ***access,*** March–April 1989] are present in HDF 3.0, plus the following new features.

An interface for basic input and output of 24-bit raster images. The routines in this interface parallel those in the HDF 8-bit raster image interface. Using these routines, you can add a 24-bit raster image set to a file, retrieve a 24-bit raster image from a file, and set the interlace scheme. (The interlace scheme is the way the red, green, and blue component values of pixels are physically grouped within the file. The color components can be grouped by color plane, scan line, or pixel.)

An interface for annotating HDF data objects and files. These routines enable you to attach text to any tagged object in an HDF file. You can attach a label, which is a short text string, or a description, which can be any amount of text. One routine also allows you to get a list of all labels in a file that are associated with a particular tag.

An interface for input and output of 8-bit palettes. With the routines in this interface you can add palettes to a file, read palettes from a file, and provide information about the palettes in a file.

Scientific dataset routines. These routines enable you to store and retrieve subsets, or slices, of scientific data and also to select optional storage formats and data types.

New utilities.

- hdfed—lets you browse in an HDF file and manipulate some of the data
- fptohdf—converts floating-point data to HDF floating-point data and/or 8-bit raster images
- r24tohdf—converts a raw RGB 24-bit image to an 8-bit RIS8 with a palette
- paltohdf—converts a raw palette to HDF format
- hdftopal—converts palette in an HDF file to raw format

HDF 3.0 is described in the new manual *NCSA HDF Calling Interfaces and Utilities*, Version 3.0, which was released in November 1989.

The source code and documentation for HDF 3.0 are available free on the anonymous ftp server at NCSA or can be purchased through the NCSA *Technical Resources Catalog.*

Although HDF 3.0 has been in beta release for several months, it may still have some bugs. If something does not seem to work the way you think it should, please contact Michael Folk by phone at (217) 244-0647 or by electronic mail at 12409@ncsavms (BITNET) or mfolk@ncsa.uiuc.edu (Internet). ▲

Caterpillar Inc. becomes seventh industrial partner

by John Patten, Assistant Director, Industrial Program

Caterpillar Inc. has signed a three-year, $3 million contract to become the seventh full partner in the NCSA Industrial Program. The world's largest manufacturer of earthmoving, construction, and materials handling equipment, Caterpillar is also a major manufacturer of diesel and natural gas engines and gas turbines.

As part of the agreement, Caterpillar scientists and engineers will be trained to use advanced computing technologies and will conduct basic and applied research on the NCSA high-performance computers.

Rich Ingram, Caterpillar supervising engineer, will be based at the center full-time and will coordinate the Caterpillar research. Some scientists will conduct their research at the center in Champaign while others will remain at Caterpillar facilities and perform their research via remote access to NCSA computers. Dee Chapman, a newly hired NCSA industrial consultant, will assist Ingram and other Caterpillar engineers.

With $10.4 billion in sales and revenues in 1988, Caterpillar sees this partnership as a major component in their plans to maintain their technological leadership.

"Computers are used extensively today to perform simulations which help to reduce the development time and cost of complex product designs and manufacturing processes," said Pierre C. Guerindon, Caterpillar executive vice president and chairman of the company's Technology Council. "Affiliation with NCSA will give Caterpillar access, training, and extensive experience with the latest supercomputers.

"This is not just an evolutionary increase in capability. Supercomputing opens entirely new doors and will allow Caterpillar engineers to gain leading-edge expertise in the solution of problems that are beyond the scope of conventional computer-aided engineering. This is an integral part of Caterpillar's mission and commitment to technological leadership," Guerindon said.

John Stevenson, NCSA associate director for the Industrial Program, welcomed Caterpillar to NCSA and stated that the partnership represents another major step in the center's goal of helping American industry meet the competitive challenge and move forward in computational science and engineering. ▲

New strategic partnership with AT&T

by AT&T Media Relations—Data Systems Group

AT&T has established a strategic partnership with NCSA to enhance use of the UNIX operating system in supercomputing environments to allow supercomputers to operate in an open system and distributed computing environment.

"This joint activity is aimed at extending the open system distributed computing architecture to serve the needs of the high-speed networks of the future," said William T. O'Shea, vice president of Product Management and Development for AT&T Computer Systems.

According to O'Shea, the company's strategic partnership with NCSA will enhance AT&T Computer Systems' networked computing strategy by incorporating supercomputers into the widespread use of open computer operating systems and universal data connectivity.

"Open operating systems, such as the UNIX operating system, are fast gaining acceptance in desktop and minicomputer environments, but are just beginning to establish themselves in the supercomputing arena," said O'Shea.

"More and more, computer users in government, industry, and education are demanding open operating systems so they can mix hardware and software from multiple vendors," O'Shea said.

"And these same users will want to work with open systems as they increase their use of supercomputers. During our first year with NCSA, we'll be developing UNIX operating system applications for supercomputing environments," he added.

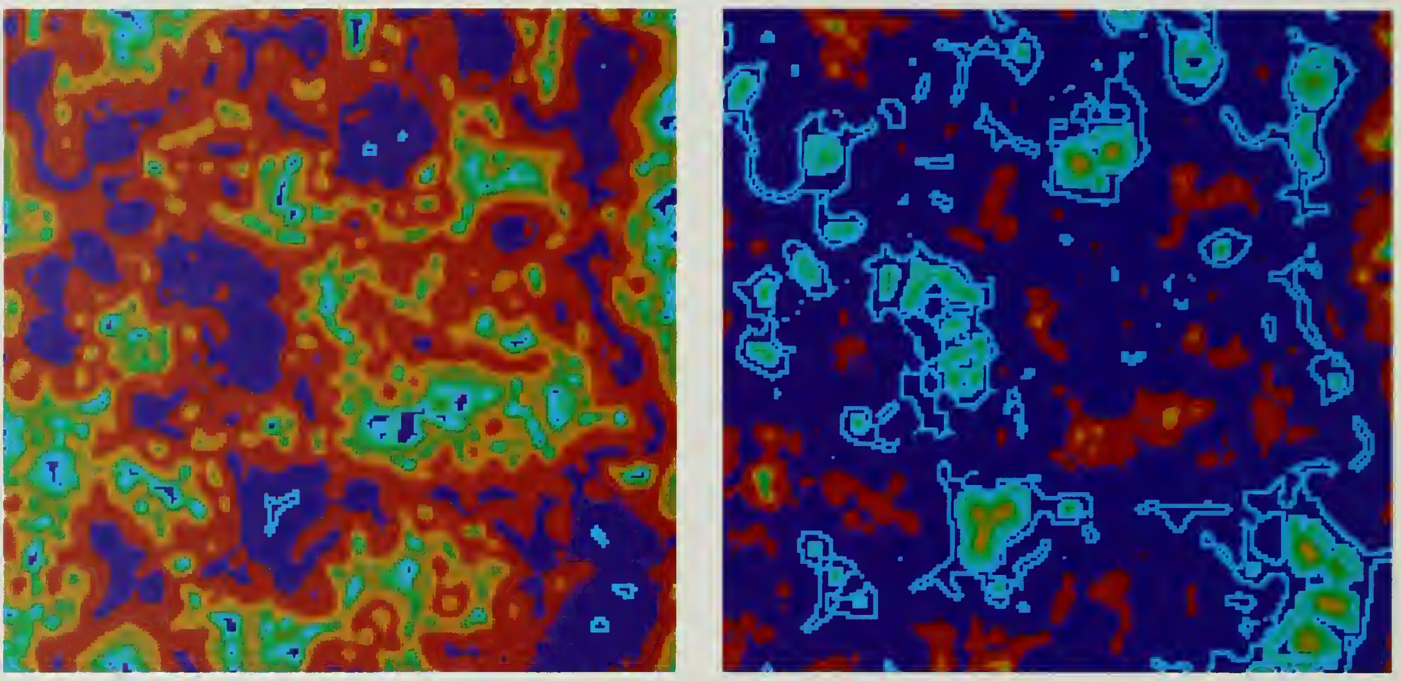
Future AT&T work at NCSA will look at ways that supercomputers could network with each other and other computing systems at rates of a billion bits per second or more.

During the first year of the three-year partnership, AT&T will contribute initial funding and provide three AT&T Bell Laboratories scientists to the facility. Funding and staffing levels for the subsequent two years are expected to grow and will be determined later.

"What is emerging is nothing less than a national information processing infrastructure for the United States," said Larry Smarr, director of NCSA. "The combination of open software systems and national high-speed connectivity will transform the research capability of America. We see AT&T as a critical leader in that transformation period." ▲

A Folk tale

by William Dwyer, Graduate Student Writer



Below. Images created by Joshua and Mike Folk that illustrate the cellular automaton known as the hodgepodge machine. Using NCSA Image, the Folks animated changes in cells. After fewer than 500 generations, the striking patterns seen here emerged, representing regions of persistent growth.

Viewers of the Apple Science '89 CD [see ***access***, July–August 1989] may have noticed images called "cellular automata" in the mathematics section and wondered what they were seeing. The images resulted from a unique father and son collaboration.

Michael Folk, senior programmer in the Software Tools Group, and his teenage son Joshua worked together on the project. Joshua supplied the initial motivation and Michael provided the advanced computer know-how.

Joshua said the project began when he asked his father to generate some averages that would produce graphs like those in an August 1988 *Scientific American* article he had read. The article describes a cellular automaton called the hodgepodge machine.

A cellular automaton can produce organized patterns that look like living things that grow and reproduce. They are actually computer models based on arrays of multivalued cells, and the hodgepodge machine, as it was named by its designers, is one of them.

In the summer of 1988, between his freshman and sophomore years in high school, Joshua read the *Scientific American* article to "break up the routine at music camp," he said. Before going to camp, he had worked with fractals at home on the family's IBM PC. At camp, the computer-generated graphics of hodgepodge machine wave patterns caught his attention because they looked like fractal patterns.

Even though the article wasn't about fractals, Joshua became interested. His father said he was talking about it when he came home from camp. "There's a section of graphs that show how certain values behave," Joshua said. "They were really regular, which I found was really amazing." Joshua enthusiastically explained how cell populations change from chaotic to organized.

The hodgepodge machine imitates certain chemical reactions quite well, too, so Joshua went to the chemistry teacher at his school to get more information about the process. He said he spent three months trying to understand the chemical reaction mechanism.

"One of the neat things about it was that it was an oscillating action," Joshua said. He was fascinated that the reaction could be duplicated on a computer, and he was interested in the relationship between the computer algorithm and the chemical reaction. But he decided not to pursue the chemistry aspect any further because "I found out I would have to do a lot more studying."

Joshua asked his father to generate some averages for plotting so he could recreate the graphs in the article. Michael used a Sun Workstation to get numbers on about 500 generations for a 100 x 100 grid of cells. Each cell represents an "automaton," an entity that was at first randomly assigned a value representing its "health." Health values range on a scale from completely healthy to dead. The health of an automaton from generation to generation depends on the health of

Folk *continued on page 18*

Seminars encourage new areas of supercomputer research

by Jarrett S. Cohen, Public Information Specialist

Supercomputers are used across a broad spectrum of research. At NCSA the three largest user groups are physics, materials science, and chemistry. Among the far smaller supercomputer user groups are history, economics, and music.

Such diversity demonstrates the strength of the technology, but few potential users—especially those in the humanities and social sciences—think of supercomputing as a research tool accessible to them.

To increase awareness among potential users of high-performance computing, the Cray Supercomputing Seminar Series features accomplished researchers who discuss how supercomputing has affected their work.

The seminars are funded by a Cray Research Inc. (CRI) grant to the University of Illinois at Chicago (UIC) as part of the UIC Graduate Workshop Program on Scientific Supercomputing [see ***access,*** May–June 1988]. Nora Sabelli, NCSA senior research scientist and assistant director for Educational Outreach as well as UIC associate professor of chemistry, is the principal investigator for the grant.

The seminars are held at both UIC and UIUC. On the Urbana campus, the seminars are presented in the Beckman Institute.

Outside funding

"We have found that we can count on the enthusiastic participation of computer industry vendors as speakers, but universities do not have the funds to sponsor such trips," Sabelli said, referring to her experience with speakers in the innovative Graduate Workshop Program. Without the support of vendors, seminars by academic researchers would be impossible.

The one-year CRI grant of $20,000 was awarded in June 1989 to support six seminars and to sponsor one UIC graduate assistantship each semester.

Expanding supercomputing

Two seminars have been given so far. Scott Ulman, of the Minnesota Supercomputer Institute and Financial Solutions Inc., spoke in November on "Fixed-Income Pricing: A Step Toward Resolving the Identification and Consistency Problems." In December Gregory McRae, of Carnegie-Mellon University, discussed "Applications of Mathematical Models in the Policy Process: Supercomputers, Smog, Acid Deposition, and Climate." [See accompanying article.]

Through this seminar series and other programs with similar aims, researchers in areas for which supercomputer use is limited are introduced more quickly to the uses of high-performance computing.

"We must provide faculty in these areas with the opportunity to discuss advances with their peers and create opportunities for collaboration," Sabelli said. "We expect our visitors, with workshop coordination, to act as catalysts for the development of new ideas, approaches, and materials."

Sabelli, in consultation with Steve Roy, coordinator of the Supercomputer Support Office at UIC, selects seminar speakers. Both UIC and UIUC faculty host the speakers' visits. Possible topics for additional seminars include city planning and architecture, linguistics, and speech recognition. Whatever the topic, these seminars are meant to broaden the use of supercomputing as a tool.

Any suggestions for topics or speakers are appreciated and should be directed to Nora Sabelli [see **NCSA contacts,** page 19]. ▲

McCrae on pollution

A key task for the 1990s is slowing or stopping damage to our environment—at a reasonable cost. Since the U.S. is spending more than $30 billion on air pollution controls, new control options need to be identified, said Gregory McRae, professor of chemical engineering and of engineering and public policy at Carnegie-Mellon.

In "Applications of Mathematical Models in the Policy Process: Supercomputers, Smog, Acid Deposition, and Climate," McRae spoke about supercomputer models in pollution control. The seminar was second in the Cray Supercomputing Seminar Series. [See article at left.]

"Mathematical models of the underlying processes provide the only technically defensible way to guide public policy making," McRae said. His own work—simulating the evolution of ozone and 30 other pollutants in the air over Los Angeles—furnished a technical basis for recent revisions to the federal Clean Air Act. NCSA director Larry Smarr has described this as the most influencial research performed at any of the NSF supercomputer centers.

McRae and colleagues Amistead Russell and Jana Miliord used Pittsburgh Supercomputer Center's CRAY X-MP/48 to solve 500,000 equations and simulate 70 test cases. One discovery refuted the widely held notion that lowering emissions automatically improves air quality. Another showed that using methanol fuel would reduce significantly the ozone produced by automobiles.

Skeptics argue that supercomputing is too expensive, a claim McRae countered by asserting, "You can pay for a Cray in a week if you can shave ten percent off the cost of air pollution control in Los Angeles."

His model has gone a long way toward doing just that. Models alone, however, are not enough. He added that scientists must learn to deal with uncertainties, evolve an iterative/integrative process, work together—as it cannot be done by one person—and couple science with policymaking by educating decision makers.

NCSA academic affiliates meet

by Lyle Rigdon, Manager, Training

The 1989 fall/winter NCSA Affiliates Meeting was held November 5–10 at the Computing Applications Building on the UIUC campus. Twenty-three representatives from academic affiliate institutions attended. The five days were packed with productive seminars, roundtable discussions, technical training lectures, and labs on a variety of topics mixed in with many open discussions of issues concerning remote users of NCSA facilities.

Several representatives from affiliate institutions spoke during the affiliates week. The following non-NCSA speakers helped make this meeting a resounding success: Steve Roy, UIC; Roger Abell, Arizona State University; Gerry McCartney, Purdue University; Tom Bouman, Southern Illinois University–Edwardsville; Janet Hartman, Illinois State University; M. Fouad Ahmad, University of Wisconsin–Milwaukee; T. J. O'Donnell, UIUC; George Francis, UIUC; and Helmut Heller, Andreas Windemuth, and Klaus Obermayer, visiting research scientists of the Beckman Institute at UIUC.

Participants' requests ranged from more intensive, advanced UNIX training and materials to more introductory videos, documentation, and on-line training. Participants also called for additional presentation materials based on the potential uses and applications of the NCSA Scientific Visualization Software Suite. Marketing materials such as videos and posters were also requested to help expand the visibility of supercomputing and its applications on their local campuses.

The spring/summer NCSA Affiliates Meeting is scheduled for April 2–6 and promises to be yet another information-packed week for representatives from NCSA affiliate institutions. ▲

Affiliates attending

Roger Abell
Arizona State University
Gary Bummer
Montana State University
Jay Crawford
Clemson University
Bruce Danner
Rose-Hulman Institute of Technology
Bryan Ferguson
Southern Illinois University–Edwardsville
Judy Halchin
Eastern Illinois University
Larry Hicks
Bradley University
Richard Jones
University of Colorado–Boulder
Paul Kramer
University of Nebraska–Lincoln
Chinh Le
Vanderbilt University
Pam Matthews
Rice University
Gerry McCartney
Purdue University
Dennis McCormick
University of Missouri–Kansas City
Jim Newton
University of Missouri–St. Louis
Allen Porter
Montana State University
Preston Prigger
The Illinois Mathematics and Science Academy
Bryan Putnam
Purdue University
Lydia Reed
University of Nevada
Steve Roy
University of Illinois–Chicago
Milind Saraph
University of Notre Dame
Bruce Tachoir
Arizona State University
Don Weihl
Southern Illinois University–Edwardsville
Bill Whitson
Purdue University

First NCSA finite element conference planned for May

by Ilhan Dilber, User Consultant

On May 14–15, 1990, NCSA is sponsoring its first Conference on Finite Element Applications in Computational Mechanics. Some of the most distinguished researchers in the finite element community will speak at this conference on the UIUC campus, including:

Ted Belythchko
Northwestern University
Jon Dantzig
UIUC
Bob Haber
NCSA and UIUC
Tom Hughes
Stanford University
Ahmed Noor
George Washington University
Mark Shephard
Rensselaer Polytechnic Institute
Tayfun Tezduyar
University of Minnesota

There will be also speakers from the NCSA academic and industrial user communities as well as other supercomputer users talking about their research or educational experiences using high-performance computing.

The registration fee is $125. To register, please return the registration form mailed with the January 1990 ***access*** or phone the registration secretary at (217) 244-7659. If you need more information regarding the conference or are interested in making a presentation at the conference, please contact Ilhan Dilber by phone at (217) 244-1973 or by electronic mail at idilber@ncsa.uiuc.edu (Internet) or 13024@ncsavms (BITNET). ▲

New NCSA academic affiliates

Arizona State University
Tempe, AZ
Bruce Tachoir
(602) 965-2900
kgbat@asuacad
and Roger Abell
aqrka@asuacad

Western Michigan University
Kalamazoo, MI
Tom Gabriele
(616) 387-5436
gabriele@gw.wmich.edu

Massachusetts Institute of Technology
Cambridge, MA
Andrew Bennett
bennett@mitva.mit.edu

Molecular modeling workshop planned for June

by Nora Sabelli, Assistant Director for Educational Outreach

A hands-on workshop on computational strategies and techniques in molecular modeling is being planned for June 11–15, 1990. The workshop will use NCSA's two teaching facilities: the Renaissance Experimental Laboratory (REL) in the Beckman Institute and the Training Facility in the Computing Applications Building. The former is equipped with 20 Silicon Graphics Personal IRIS workstations for 3D visualization, the latter with 20 Macintosh IIcx personal computers for 2D visualization and supercomputer access.

Topics to be covered include ab initio and semiemperical calculations, force fields parameterization, free-energy calculations, and solvation effects. Guest speakers from academia and industry will talk on computational strategies, comparisons between methods and parameterizations, and general troubleshooting for common computational bottlenecks.

Participants will work on their own research and computation problems in teams and will be able to interact with the speakers in informal discussions.

Watch for more information in future issues of ***access,*** or contact one of the three organizers: Nora Sabelli [see **NCSA contacts,** page 19]; Joe Golab by phone at (217) 244-2756 or electronically at 12688@ncsavms (BITNET) or jgolab@ncsa.uiuc.edu (Internet); or Mike Heathman by phone at (217) 244-7687 or electronically at heathman@ncsa.uiuc.edu (Internet). ▲

Online notes

New and updated online information

by Will Ridenour, Online Documentation Editor

The following help files, documents, and man pages have been added or updated as of January 22, 1989. This list updates the November–December 1989 NCSA *Online Documentation on the Cray Systems.* For a copy of this publication, contact Orders for User Publications and NCSA Software [see **NCSA contacts**, page 19].

UNICOS help files

Topic name	**Description**
calendar	*scheduled NCSA events*
holidays	official university holidays
consulting	consulting office schedule
contacts	*whom to contact for various problems*
coordinators	software research area contacts
affiliates	NCSA affiliate contacts
consult	consulting office location and phone
software	*the latest list of software on NCSA machines*
graphics/ncar	information about the NCAR Graphics package
unicos	*information about UNICOS at NCSA*
vi	information about the vi editor under UNICOS

To access a help topic, enter **`help topic`** where topic is the name of the topic you wish to view.

UNICOS documents

Document name	**Description**
specfun	information about the SPECFUN mathematical library
pascal	information about the CRI Pascal compiler
update	information about CRI's UPDATE file maintenance program
datalink	*back issues*
nov-dec.89	the November–December 1989 issue of ***data link***

Online *continued on page 12*

***Online** continued from page 11*

sep-oct.89	the September–October 1989 issue of ***data link***
unicos5	*CRI's UNICOS 5.0 release notes*
front	front matter for UNICOS 5.0 release notes
sec[1-8]	Sections 1–8 of the UNICOS 5.0 release notes

To access an online document, change directories to /usr/local/doc and enter `more docname` where docname is the name of the document you wish to view.

UNICOS man pages

NOTE: Man pages marked with a superscript x are available on the CRAY X-MP/48 only. Those marked with a superscript 2 are available on the CRAY-2 only. The man page descriptions below match word for word the online descriptions.

Man page name	Description
ansys^{2}	Finite Element Analysis Program, version 4.3a
areas	creates an area map from a set of edges
autograph	draws curves or families of curves
cgmtrans	NCAR CGM translator
colconv	converts a color specification given in hue, lightness, and saturation color space to values in the RGB color space
conran	contours irregularly spaced data, labeling lines
conraq	contours data, no labeling
conras	contours data, lines smoothed, crowded lines removed
conrcq	contours 2D arrays, no labeling
conrcspr	contours 2D arrays, lines smoothed, crowded lines removed
conrec	contours 2D arrays, labeling contour lines
ctrans	a CGM translator
dashchar	software dashed-line package with character capability
dashline	software dashed-line package
dashsmth	software dashed-line package with character capability and smoothing
dashsupr	software dashed-line package with character capability, smoothing, and the capability of removing crowded lines
emacs	programmable, extensible text editor
ezmap	plots world/regional border outlines
ezmapa	allows EZMAP output redirection to AREAS routines
fluent	general-purpose program for modeling fluid flows
fontc	fontcap preprocessor for NCAR Graphics
fontcap	NCAR Graphics font definition file
ftrans	NCAR CGM translator
graphc	graphcap preprocessor for NCAR Graphics
graphcap	NCAR Graphics graphic device definition file
gridal	draws background grids
hafton	halftone pictures of 2D arrays
histgr	plots histograms
isosrf	isosurfaces from 2D arrays, hidden lines removed
isosrfhr	isosurfaces from high-resolution 3D arrays
marc^{x}	general-purpose finite element analysis program
ncargcc	command for compiling C code that uses NCAR Graphics
ncargex	script for executing NCARG programs
ncargf77	command for compiling f77 code that uses NCAR Graphics
ncargintro	NCAR Graphics overview
ncargtest	create, compile, and link a program that uses an NCAR Graphics utility
nprint	provides UIUC campus printing and plotting capabilities
plotchar	character plotting package
plt	user interface for NCAR metacode translators
pwritx	fancy characters plotting
pwrity	character plotting plots
pwrzi	plots characters in 3D with ISOSRF
pwrzs	plots characters in 3D with SRFACE
pwrzt	plots characters in 3D with THREED
scrdiff	save, restore, and manipulate scratch directories
scrget	save, restore, and manipulate scratch directories
scrls	save, restore, and manipulate scratch directories
scrput	save, restore, and manipulate scratch directories
srface	3D plot of functions with 2 variables
specfun	a library of special function software
strmln	draws a streamlined representation of a flow field
threed	3D line drawing package
tsock^{2}	UltraNet socket-based network exerciser
ugraf^{2}	accesses Ultra Graphics Display Device
unetcf^{2}	configure UltraNet network
unetdb^{2}	control UltraNet kernel printout
unet_ioctl^{2}	Ultra Network Technologies driver interface ioctl's
unet_trace^{2}	Ultra Network Technologies in-kernel trace macro
velvct	draws 2D velocity fields
zetavu^{2}	read Zeta GML files

To access a UNICOS man page, enter `man manpage` where manpage is the name of the man page you wish to view. ▲

Advisory Board meets

by Virginia Hudak-David, Assistant Director, Administrative Affairs

The NCSA Advisory Board held its semiannual meeting at Allerton Park on December 11 and 12, 1989. The rural retreat is located some thirty miles from the UIUC campus.

Following presentations by NCSA management, senior NCSA administrators and board members stayed at Allerton after a working dinner. Discussions continued on the second day.

The board first heard presentations from NCSA Deputy Directors Jim Bottum and Karl-Heinz Winkler and from the center's associate directors, setting the stage for the following day's closed session with NCSA Director Larry Smarr and the deputy directors. Senior staff in Operations, Planning, and Client Relations provided detailed updates on finance and administration and on the academic, state, and industrial programs. Science, Technology, and Education program initiatives were described, including information on operations and facilities, systems and software, and applications. NCSA's proposed Corporation for National Research Initiatives (NRI) project was also summarized.

The second day's closed session was devoted to frank discussions about various issues raised during the presentations the previous day. The board reviewed progress of the center's internal reorganization that began in the summer of 1989, about the time of the board's last meeting. Other topics discussed were NCSA's role in education, the high-performance computing initiative, financial planning, space, and the supercomputer upgrade path.

The NCSA Advisory Board will meet again in the summer of 1990. ▲

Training dates

March 5–9	New User Training
April 2–6	Affiliates Training
April 23–27	New User Training
May 14–18	New User Training
June 4–8	New User Training

Note: Dates are subject to change. Class size is limited. You must register to attend NCSA training.

To register: Academic users, contact Kendra Reasor at (217) 244-1100. Industrial partner users, contact your representative at NCSA.

Additional information: Contact Janice Knapp-Cordes by phone at (217) 333-0085 or by electronic mail at janicek@ncsa.uiuc.edu (Internet) or 13036@ncsavms (BITNET).

Advisory Board members

Ron Deiss
Chairman
Deputy Director of NAS, NASA Ames Research Center
Riaz Abdulla
Industrial Program Representative
Eli Lilly and Company
Kenneth Bishop
Academic Affiliate Representative
Professor of Petroleum Engineering, University of Kansas
Jonathan Dantzig
Associate Professor of Mechanical and Industrial Engineering, UIUC
Ernest Davidson
Professor of Chemistry, Indiana University
Charles R. Evans
Assistant Professor of Physics and Astronomy, University of North Carolina–Chapel Hill
Arthur Freeman
Professor of Physics, Northwestern University
Eric Jakobsson
Associate Professor of Bioengineering, UIUC
Lawrence Landweber
Professor of Computer Science, University of Wisconsin
Bernard O'Lear
Manager of Systems, National Center for Atmospheric Research
Larry Ray
Industrial Program Representative
Research Scientist, Eastman Kodak Company
Jon Sauer
Adjunct Professor, Optoelectronics Computing Systems Center, University of Colorado
John Steele
Director of Computing Center, Purdue University
Robert Wolff
Senior Research Scientist, Applications Technology Department, Apple Computer Inc.
Paul Woodward
Professor of Astronomy, University of Minnesota

Recent allocations to NCSA supercomputers

by Patricia Wenzel, Manager, User Administration

At the December meetings of the Peer Review Board (PRB) and Small Allocation Committee (SAC), it was announced that the CRAY-2 system at NCSA is fully allocated. Therefore, CRAY-2 service units (SUs) allocated at the December meetings will be added to the system no sooner than March 1990, but CRAY X-MP/48 and CM-2 allocations were added immediately.

Projects approved at the December allocations meetings are listed alphabetically by principal investigator.

Peer Review Board meeting—December 14, 1989

Jan E. Almlof, University of Minnesota, *Development and Applications of Direct Methods for Electronic Structure Calculations*, CRAY-2, 875 SUs.

Alvin Bayliss, Northwestern University, *Numerical Study of Pattern Formation in Combustion*, CRAY X-MP/48, 400 SUs.

Ronald E. Cohen, Naval Research Laboratory, *First Principles Lattice Dynamics of Oxides*, CRAY-2, 1500 SUs.

Jennifer M. Cram, Colorado State University, *The Numerical Simulation and Analysis of the Initial Development of a Prefrontal Squall Line*, CRAY-2, 140 SUs.

Clinton N. Dawson, University of Chicago, *Flow in Porous Media*, CRAY X-MP/48, CRAY-2, 99 SUs.

Rodney O. Fox, Kansas State University, *Dynamics of Poorly-Mixed Chemical Reactions in a Flow Reaction*, CRAY X-MP/48, 50 SUs.

Dimitri Gidaspow, Illinois Institute of Technology, *Hydrodynamics of Circulating and Bubbling Fluidized Beds*, CRAY X-MP/48, 100 SUs.

Thomas Halsey, University of Chicago, *Problems in Electrochemistry*, CRAY-2, 50 SUs.

John F. Hawley, University of Virginia, *Numerical Astrophysics*, CRAY X-MP/48, CRAY-2, 430 SUs.

Houk/Armstrong, University of California–Los Angeles, *Theory and Modeling of Organic Reactions and Stereoselectivity*, CRAY X-MP/48, 250 SUs.

Detlef Hohl, UIUC, *Molecular Dynamics and Density Functional Theory: Static and Dynamical Properties of Main Group V and VI Clusters, Liquids, and Amorphous Solids*, CRAY X-MP/48, CRAY-2, 700 SUs.

Frederick Warren King, University of Wisconsin–Eau Claire, *Precise Energy-Level Calculations for Three-Electron AtomsLitch*, CRAY X-MP/48, 160 SUs.

John B. Kogut, UIUC, *Field Theory Simulation on a Connection Machine*, CM-2, 200 SUs.

J. Bruce Litchfield, UIUC, *Measurement of Transient Moisture Profiles and Structural Changes Using 3D NMR Microscopy*, CRAY-2, 100 SUs.

William H. Miller, University of California, *Quantum Reactive Scattering*, CRAY-2, 200 SUs.

Dwight R. Nicholson, University of Iowa, *Solitons and Ionospheric Heating*, CRAY-2, 150 SUs.

David Wallace Onstad, UIUC, *Parallel Processing and High-Dimensional Graphical Analysis of Numerical Models Concerning the Biological Control of Insects*, CRAY X-MP/48,CM-2, 120 SUs.

Ian D. Parsons, UIUC, *The Stability of Stiffened Composite Shells: Numerical Investigations and Algorithm Development*, CRAY X-MP/48, 50 SUs.

Roger A. Pielke, Colorado State University, *Impact of Regional Flow Patterns on Thermally Induced Mesoscale Circulations*, CRAY-2, 201 SUs.

James R. Rice, Harvard University, *Stress Accumulation and Its Seismic Release in Shallow Fault Zones*, CRAY X-MP/48, 320 SUs.

Jonathan R. Sapirstein, University of Notre Dame, *Weak Interactions in Atomic Physics*, CRAY X-MP/48, CRAY-2, 250 SUs.

Klaus Schulten, UIUC, *Large-Scale Simulations of Adaptive Maps and Related Neural Network Algorithms*, CRAY-2, CM-2, 850 SUs.

David N. Seidman, Northwestern University, *Monte Carlo Simulations of Solute-Atom Egregation at Internal Interfaces in Dilute Alloys Mainly the Effects of Chemistry*, CRAY X-MP/48, CRAY-2, CM-2, 247 SUs.

Harrell Sellers, NCSA, *Transition Metal Chemistry—Catalysis*, CRAY-2, 400 SUs.

Donald Scott Stewart, UIUC, *Numerical Simulations of Detonation Dynamics*, CRAY X-MP/48, 200 SUs.

Wei Shyy, University of Florida, *Numerical Prediction of Transport Characteristics and Macrosegregation of Superalloy Processing*, CRAY X-MP/48, 75 SUs.

S. Y. Tong, University of Wisconsin–Milwaukee, *Determination of Surface and Interface Structures by Local and Long-Range Order Diffraction Techniques*, CRAY X-MP/48, CRAY-2, 480 SUs.

Robert Wilhelmson, UIUC, *Convection / Storms / Tornadoes*, CRAY-2, 600 SUs.

Henry W. Wyld, UIUC, *Simulations in Lattice Gauge Field Theory*, CRAY X-MP/48,CM-2, 450 SUs.

Small Allocation Committee meeting—December 10, 1989

Dennis N. Assanis, UIUC, *Development of an Improved Combustion Model for Use in a Multidimensional Engine Simulation*, CRAY X-MP/48, CRAY-2, 90 SUs.

Robert S. Averback, UIUC, *Molecular Dynamics Studies of Ionited Cluster Beam Deposition*, CRAY X-MP/48, 95 SUs.

Gunadya Bandarage, University of Colorado, *Harmonic Generation / Nonlinear Effects in Laser-Atom Interactions*, CRAY X-MP/48, 80 SUs.

Samuel Bernstein, Energy International Inc., *Extended-Throat Venturimeter for Online Measurement of Gas-Solid Flow*, CRAY X-MP/48, 10 SUs.

Semion Gutman, University of Oklahoma, *Instabilities, Pattern Formation, and Turbulence in Flames*, CRAY-2, 60 SUs.

Richard Lahey, Rensselaer Polytechnic Institute, *Analysis of Boiling Using a Multidimensional Finite Element Method*, CRAY X-MP/48, 20 SUs.

Don Q. Lamb, University of Chicago, *Statistical Analysis of the Angular Distribution of Neutrinos Observed from SN 1987A*, CRAY X-MP/48, 65 SUs.

Shen C. Lee, University of Missouri–Rolla, *Turbulence Modeling for Transition Studies*, CRAY X-MP/48, 20 SUs.

John W. Leonard, Oregon State University, *Nonlinear Interaction of Water Waves and Deformable Structures*, CRAY X-MP/48, 10 SUs.

Alan R. Mickelson, University of Colorado, *Inverse Methods in Guided Wave Optics*, CRAY X-MP/48, 85 SUs.

Ignacy Misztal, UIUC, *Estimation of Variance Components Using Sparse Matrix Techniques*, CRAY-2, 50 SUs.

Roger A. Pielke, Colorado State University, *Influence of Anthropogenically Increased Cloud Albedo on Global Climate*, CRAY-2, 37 SUs.

Umberto Ravaioli, UIUC, *Simulation of Semiconductor Lasers (MINILASE)*, CRAY X-MP/48, 20 SUs.

Michael Richman, Illinois State Water Survey, *Diagnostic Studies of Growing Season Rainfall Fluctuations in Central North America*, CRAY-2, 40 SUs.

Dilano Kerzaman Saldin, University of Wisconsin–Milwaukee, *Holographic Low-Energy Electron Diffraction*, CRAY X-MP/48, 5 SUs.

James Truran, UIUC, *Research in Astrophysics*, CRAY X-MP/48, CRAY-2, 90 SUs.

Almon Turner, University of Detroit, *Role of C1-NOx,F-NOx Type Molecules in Ozone Depletion*, CRAY X-MP/48, CRAY-2, 99 SUs.

G. E. O. Widera, UIC, *Application of Finite Element Analysis in Pressure Vessel and Piping*, CRAY X-MP/48, 5 SUs. ▲

Allocation statistics

	SAC Meeting	PRB Meeting
Number of Proposals	**21**	**32**
CRAY X-MP only	12	6
CRAY-2 only	5	14
CM-2 only	0	1
Combination of above	4	11
Fully allocated	13	19
Partially allocated	4	9
Deferred	4	4

	SAC Meeting			PRB Meeting		
	X-MP	**CRAY-2**	**CM-2**	**X-MP**	**CRAY-2**	**CM-2**
Hours requested*	890	465	0	3249	7208	3980
Percent allocated^	62%	66%		97%	77%	22%

* These figures reflect what is allocated for the coming year only. They do not include service units for the second and third years of multiyear requests.

^ Some allocations were deferred pending requests for additional information from researchers. These will be acted on before the next meeting, if possible. Deferred allocations are not included in these figures.

Visitors from Japanese academic computing centers

by Fran Bond, Technical Editor

Recently representatives from Japan's academic computing centers visited NCSA as part of a tour of NSF-sponsored supercomputing centers.

Dr. Katsuhiko Miyoshi, professor and manager of the R&D Division of the Hokkaido University Computing Center, headed the delegation. The purpose of the visitors' mission, said Miyoshi, was to take steps to form a worldwide supercomputer center in the early nineties that would include representatives from Japan, Europe, and the United States.

While at NCSA, the visitors toured the Renaissance Education Laboratory (REL) at the Beckman Institute as well as the Cray supercomputing facility in the Astronomy Building. They also met with representatives of the center's networking, visualization, and software groups.

Miyoshi and Dr. Iida Noriko, associate professor of the National Center for Science Information System (NACSIS) in Tokyo, spoke on Japan's scientific networking and academic computing services respectively.

The eight visitors were from member institutions of Japan's National Academic Computing Service. Governed by the Ministry of Education, the centers have been networked on Japan's Science Information Network since 1987. Early last year the network was connected to the U.S. via satellite. According to Miyoshi, supercomputers were introduced to Japan's university computing centers in 1985.

University computing centers situated at Tokyo, Hokkaido, Osaka, Kyoto, and Sendai were represented in the delegation together with the member from NACSIS. ▲

Dr. Katsuhiko Miyoshi (far right) led a delegation from Japan's academic computing centers in a visit to NCSA.

A note for GAUSSIAN86 users

by Joe Golab, Applications Scientist, Computational Chemistry Group

GAUSSIAN88 is installed on both NCSA Cray systems in the directory /usr/local/apps/chem/gaussian88. GAUSSIAN88, a connected system of programs for performing semiempirical and ab initio molecular orbital calculations, is the latest version of the GAUSSIAN computational chemistry application distributed by Gaussian Inc. and represents further development of the GAUSSIAN70, GAUSSIAN76, GAUSSIAN80, GAUSSIAN82, and GAUSSIAN86 systems already published.

Gaussian Inc. distributes and supports only the latest version of the GAUSSIAN program for each computer system. With the announcement of GAUSSIAN88 for UNICOS Cray Systems, the corresponding implementation of GAUSSIAN86 has been discontinued by Gaussian Inc. As a result, in March 1990 GAUSSIAN86 will be removed from the NCSA CRAY X-MP system. The exact date is tentative but you should prepare *now* for the fact that GAUSSIAN86 will no longer be available on the CRAY X-MP system in the second quarter of 1990.

Documentation for GAUSSIAN88, Revision C Version (dated Friday, September 23, 1988) can be ordered by calling Orders for User Publications and NCSA Software [see **NCSA contacts,** page 19]. ▲

***Expanding** continued from page 5*

problems in just one or two dimensions.

"In some ways, people have been searching for this kind of artificial intelligence, mathematically, to build into an algorithm. But if you look numerically at where computer technology is going, a lot of artificial intelligence can now be supplied by actual engineers at their workstations—they have so much more interactive ability due to the progress of the software through interfaces and immediate visualization. This whole area is really new, and I think it will lead towards another way people view simulation software. The entire process cuts down on a lot of time and creates better understanding of what the solution is really giving you."

Using the tools in multiple areas

Raefsky has used NCSA software in geophysical and mechanical engineering as well as in electrical engineering. In geophysics, he has worked with Dr. Gregory Lyzenga to model the San Andreas fault [see **access,** November–December 1989] and more recently with Scott King, a graduate student at California Institute of Technology, on the convection in the earth's mantle. Raefsky outlines their research: "Essentially over geologic time scales, the earth's mantle flows as a creeping fluid; thermal forces within the earth drive this fluid. NCSA Image has been extremely valuable in creating the visualization of the flow within the earth.

Raefsky goes on to explain the usefulness of other tools in the NCSA Scientific Visualization Suite: "Another really valuable tool has been NCSA Layout because we've been able to capture some interesting frames from the animation and annotate those to point out the interesting parts. Recently we've been combining the NCSA Image and NCSA Layout tools. For example, we can run a video created in NCSA Image in which you'll see some animation of fluid flow within the earth. At a certain point, up will pop a slide containing noteworthy graphics that are also part of the animation sequence. The video animation stops and in essence says, 'Look at this formation, look at this structure.' You can have that particular slide all in text with arrows and with the particular palettes that you want to use. After the slide's pertinent information has been pointed out, you can continue the animation.

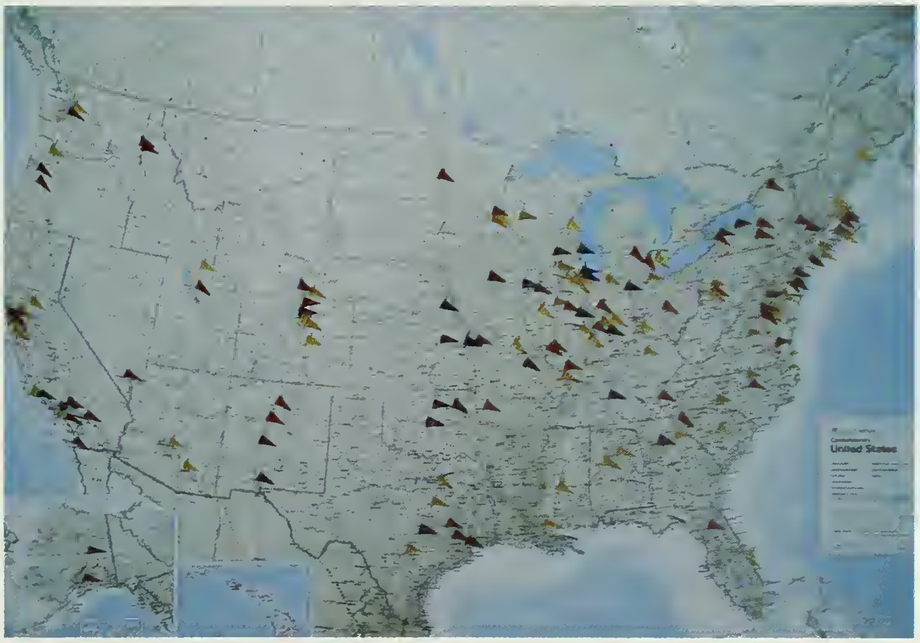
"NCSA PalEdit has also been extremely valuable to us. After fiddling around in NCSA ImageTool, we get an idea of the kinds of palettes that really bring out the science we're trying to understand. We then can bring those palettes into PalEdit, explore their structure, and from that try to create other palettes that we might not have been able to do before. I guess what really amazes—and interests—us is that, by using different colors, you get such a different view of the same set of solutions and bring out different features of the flow that you wouldn't normally see."

Helping with presentations

Recently Raefsky and his associates have submitted a proposal to the Defense Advanced Research Project Agency (DARPA) using a videotape created with NCSA software. He says that the tools were "very useful and actually powerful in presenting the proposal." He adds that NCSA Image has now become an integral part of all their presentations.

In late January, Semiconductor Research Corporation sponsored a hands-on workshop at Stanford entitled "Integrated Technology Modeling for IC Process and Device Design." A large number of industrial researchers either attended the workshop in person or watched it nationwide over the Stanford Instructional Television Network. NCSA Image and ImageTool for the Macintosh and Sun Workstation were key parts of the workshop. Also aired were segments from a Stanford videotape showing people using NCSA software tools to create animations. ▲

NCSA user sites



The small flags are color coded to indicate the cumulative number of NCSA computer users, ranging from white for one user per site to red for 60 or more users per site. As of January 22, NCSA academic and industrial users totaled 4,475 at 290 sites.

Software continued from page 3

work emphasizes an individual's research.

Jacobs, assistant professor of plant biology at UIUC, says that GelReader "will be a terrific value to molecular biologists." According to Jacobs, molecular biologists often deal with two-dimensional images that are displayed on X-ray film, photographs, or synthetic membranes. Scientists photograph the images and place the results in research papers and in published articles. Although "there is a quantitative aspect to these images, we rarely use anything very sophisticated to show that quantification. We just lay a ruler on top of images or even photograph them with a ruler in the picture.

"Sophisticated analysis costs at least $25,000, and truly excellent analytical hardware/software combinations begin at $100,000," Jacobs adds to explain why rulers are often used instead. "A desktop scanner costs $1000, most people already have microcomputers, and GelReader is free. Thus, accessibility to technology is a plus for NCSA and GelReader."

The traditional approach has limitations, Jacobs feels. If biologists were to use software that could digitize and analyze the images and also store them in a database for easy access and comparison, he says biologists would "embrace it enthusiastically." NCSA GelReader can fulfill these needs.

Jacobs also discusses the effect of NCSA GelReader on the single scientist: "My interest in this project has been and continues to be development of software for everyone; that is, for the molecular biologist in the modest laboratory. Molecular biology generally doesn't require million-dollar hardware. A lot of people are doing it on pretty small budgets, and even those people can be terrifically benefited by a program like this—so can students, for that matter. It's something students could use to analyze the data they've generated in a laboratory class. So it's not something that requires input data from a 5 million dollar supercomputer. The input data comes from equipment you use in the laboratory that will cost you a couple hundred dollars and that every molecular biologist in the country is using."

Once GelReader has received wide exposure, Jacobs predicts that "NCSA is going to have to set up a special person to handle the influx of requests for this program. I really think this will be very popular. . . . I think when biologists see what this thing will do they'll say, 'Well, wait a minute! We really have been messing with rulers for too long.' " ▲

Folk continued from page 8

its nearest neighbors. In other words, the sicker its neighbors, the sicker the automaton becomes.

After so many generations, regions of healthy and unhealthy automatons establish themselves in patterns that remain relatively stable through succeeding generations. These are the patterns mentioned before that resemble the balances reached in certain chemical reactions.

But the Folks did not get the expected patterns at first. They looked at the article again and found that they would need more generations. Five hundred generations with the 100 x 100 grid take about 25 million calculations on a computer. To do the calculations for more than 500 generations, Michael decided to move over to the CRAY-2 during its friendly user period.

"Then we wanted to get pictures," Joshua said. "That took a while. Dad did that. We were trying to get these pretty *Scientific American* pictures."

Michael used C programs under the UNICOS operating system to generate the raw data. Then he used programs from the NCSA Scientific Visualization Software Suite [see ***access,*** July–August 1989]—in particular, NCSA DataScope and NCSA Image—to generate and manipulate the images.

"These programs take sets of floating-point numbers and convert them to a scale of 0 to 255," Michael explained. "You assign each one a color. You just look at that array on the screen. The interesting thing is that, after enough generations, the patterns appear." The patterns stabilized after about 1,000 generations. He explained how to manipulate the palette to "pull out certain types of information," in this case, to show the regions of varying health of automatons.

Michael also used the project for debugging the Hierarchical Data Format (HDF) utility [see ***access,*** January–February 1989 and page 4 of this issue], a part of the software suite that he developed. His most recent plan was to take advantage of the friendly user period on the Connection Machine (CM-2) at NCSA [see ***access,*** September–October 1989] to improve the cellular automaton grid setup.

The problem is that, for a two-dimensional grid, the cells at the edges do not have neighbors all around them. The patterns are affected by this nonuniformity, Michael said. The remedy is to wrap the grid so that the edges meet to form a toroid, a donut shape. He would like to use the Connection Machine and assign each cell to a processor. A 100 x 100 grid of cells would use only 10,000 of the 32,768 processors available.

Joshua, a junior in high school this year, is uncertain how this project will affect his future study. He doubts that he will major in computer science in college, but chemistry is a possibility. "I really have no idea what I'm going to do," he said. "There are so many interesting things." ▲

Scientific visitors

Thomas Bouman
August 30, 1989–August 15, 1990
Southern Illinois University–Edwardsville
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by Diane Cook, Student Consultant

GAUSSIAN88 available on the NCSA Cray systems
by Joe Golab, Applications Scientist

MM2(87) and MINP available on the NCSA Cray systems
by Joe Golab, Applications Scientist

IMSL library source code access
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Science

From biological photodiodes to brain structure

by Kathleen Robinson, Science Writer

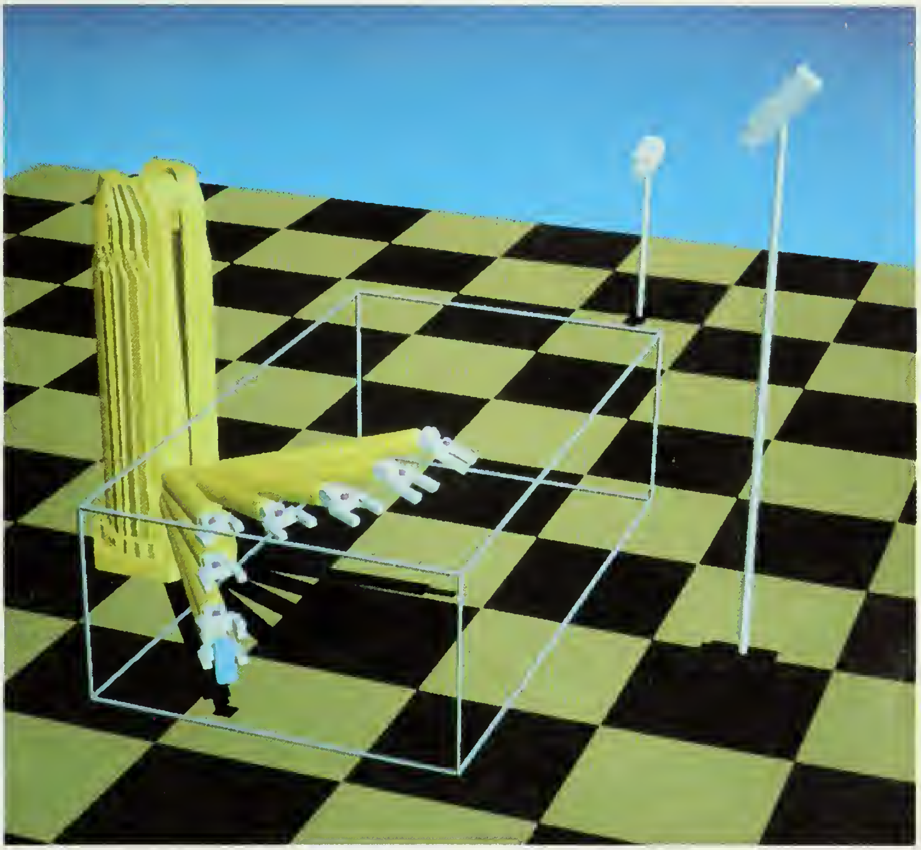
Dr. Klaus Schulten, UIUC theoretical physicist and a staff member at the Beckman Institute, heads the interdisciplinary Theoretical Biophysics Group that is studying biological systems from the molecular level to the highest levels of biological organization, as realized in the brain. Schulten's group applies the tools of physics, chemistry, biology, and computer science in their research.

"The reason we need supercomputers is very simple," Schulten says. "Biological systems are complex. Biological macromolecules contain tens or hundreds of thousands of atoms, and to describe them you need more than pencil and paper. My pencil is the Cray—it allows me to think about these complex systems."

In addition to NCSA's CRAY-2 system, Schulten and his group use the recently acquired Connection Machine [see ***access***, September–October 1989]. They also have built a transputer that will be available to other NCSA users. "The transputer is really two systems," explains Helmut Heller, a member of Schulten's research group. "One system has 18 nodes, and the other has 12. We can combine them to make one transputer with 30 nodes. Each node has 4 Mbytes of memory. We use the transputer for running our molecular dynamics software to simulate very large biological molecules."

They have written a molecular dynamics simulation code that can be used with the codes CHARMm and XPLOR. "We put the numerically intensive parts on our transputer," explains Heller, "and then go out to those other programs for doing analysis."

***Biological** continued on page 3*



A robot arm that learned to grasp objects (left). A typical sequence of arm configurations is shown as the robot grasps the blue cylinder at the middle left of the foreground (see page 14). (Courtesy Theoretical Biophysics Group)

Because of a power outage due to an ice storm, the CRAY X-MP/48 and the CRAY-2 systems were down from 8:02 p.m. CST on February 14 through 8:26 a.m. CST on February 17. We regret any inconvenience this may have caused you.

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New names at NCSA

Interdisciplinary Research Center (IRC) is now **Interdisciplinary Research Program** (IRP).
Software Development Group (SDG) is now **Software Tools Group** (STG).
Visualization Development and Services Group (VDSG), formerly the Scientific Visualization Program and Media Services Group, is now **Visualization Services and Development** group (VSD).

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Abbreviations

CRI	Cray Research Inc.
IRP	Interdisciplinary Research Program of NCSA
NCSA	National Center for Supercomputing Applications
NSF	National Science Foundation
OPCR	Operations, Planning, and Client Relations
STE	Science, Technology, and Education
UIC	University of Illinois at Chicago
UIUC	University of Illinois at Urbana-Champaign

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Biological *continued from page 1*

Biological photodiodes

Schulten's first work with NCSA facilities involved the photosynthetic reaction center of *Rhodopseudomonas viridis* [see ***access***, July–August 1987]. This protein plays a vital role in the biosphere, allowing plants to convert the energy of sun-light into electrical energy which they then use to metabolize sugar and starch. The photosynthetic reaction center is, in effect, a biological photodiode. The structure of this protein (the arrangement of its 12,637 atoms) has been established through experimental methods such as x-ray crystallography. Working with Schulten on this project are Heller, Markus Tesch, and Dr. Marco Nonella. They used the structural data as a starting point in molecular dynamics simulations.

Schulten's work not only relied heavily on NCSA's computational power, but on its visualization facilities as well. Says Schulten, "The results of these enormous calculations can only be handled by the human mind if we use the *eye* as the information channel." As a result of the reaction center studies, researchers have a better understanding of how this biopolymer so efficiently converts sunlight to stored energy.

DNA and anticancer drugs

In another project, Schulten and Klaus Boehncke, another member of the Theoretical Biophysics Group, are pursuing a collaboration with Dr. Andrew Wang, x-ray crystallographer and UIUC professor of physiology and biophysics. According to Schulten, "We are particularly interested in the interaction between DNA (genetic coding molecules) and certain anticancer drugs. Wang uses x-ray crystallography to determine the structure of the DNA when it is bound to a particular anticancer drug. We then use the structural data in molecular dynamics simulations."

Schulten's group is studying how the drug binds to DNA and the degree of specificity that is necessary. This work is important both as basic biochemistry and because it may lead to the design of more effective drugs to fight cancer.

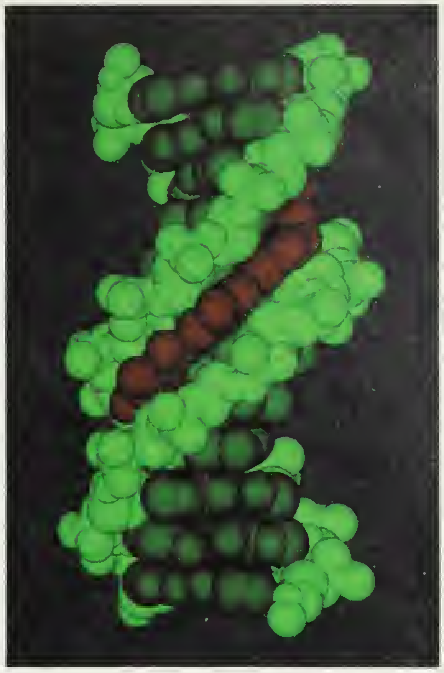
NMR imaging microscope

Working up the ladder of complexity in biological systems to the study of cells, the next project Schulten describes is a collaboration with Dr. Paul Lauterbur. Lauterbur, director of the UIUC Biomedical Magnetic Resonance Laboratory [see page 4], pioneered the technique of nuclear magnetic resonance (NMR) imaging. This technique allows researchers to "view" a tissue's interior noninvasively—by first orienting nuclear spins, such as those of water, through exposure to a strong magnetic field, then applying pulses of radio frequency magnetic fields and recording the signals subsequently emitted by the different types of nuclei. Daniel Barsky and Benno Puetz are working with Schulten on this project. They simulate the measuring process used in NMR imaging to investigate how chemical diffusion—which occurs naturally in tissues—affects the resolution of the images and their interpretation.

Schulten explains, "We simulate the measuring process. For this purpose we assume a certain tissue situation and simulate water diffusing around. We simulate how the spins react to the measuring process and then see what results. Since we know what the tissue situation is, we can relate the constructed image back to the known status of the tissue. Diffusion distorts the images, and we are learning to account for that."

Connection Machine and brain

Yet a fourth facet of Schulten's work involves simulating the multicellular systems involved in sensory perception, using the Connection Machine to represent part of a monkey's brain. Dr. Helge Ritter and Klaus Obermayer are the primary researchers on this project. As Schulten explains, "In certain monkeys, the size of the brain tissue that represents the monkey's hand is a few square millimeters in area and contains several hundred thousand neurons. These neurons have several million interconnections and connections with the body surface. "Actually," he adds, "the numbers are still a little too large, but we managed to fit a model of a reduced part of the monkey's cortex into the Connection Machine."



Complex of a DNA molecule with anticancer drug dystomycin. Drug is in red, bound in the so-called minor groove of the DNA molecule (in green). Two shades of green distinguish the two strands of DNA that form the famous double helix. Image produced using QUANTA on a Silicon Graphics 220 GTX. (Courtesy Theoretical Biophysics Group)

Experimental work done by others showed that when one finger of a monkey is amputated, after some period of time the connections to the somatosensory cortex that once represented the amputated finger change to represent the two neighboring fingers. Basing their simulation on the now widely accepted assumption that neurons have a tendency to alter the strength of their connections through repeated use, Schulten's group was able to show that nerve tissue can self-organize the representation of the monkey's hand. Says Schulten, "It is not necessary that the representation—the connections of the receptors to the cortex—be genetically prewired. Rather, they can establish themselves according to genetically determined rules.

"Since this modest beginning, we have now started to look at a more complicated neural system, the eye. Our simulations show the emergence of a connection pattern between the receptors of the retina and the optical cortex which is very similar to that

Biological *continued on page 14*

Imaging advances

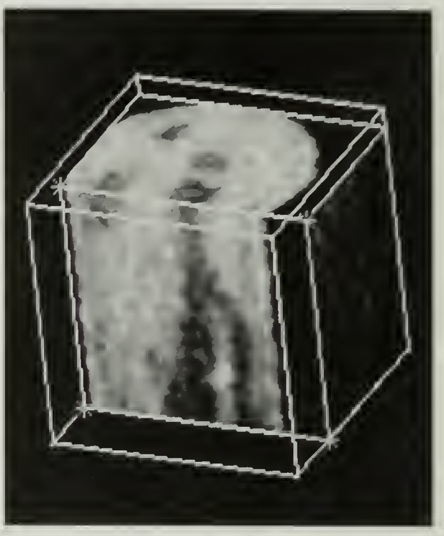
by Kathleen Robinson, Science Writer

Nuclear magnetic resonance (NMR) imaging is a noninvasive method for viewing tissues that does not use ionizing radiation—which makes the imaging process different from CAT scans. In NMR imaging, a large magnet surrounds the subject or tissue sample with a constant field, causing the nuclear spins of the atoms to become aligned. Pulses of radio frequency magnetic fields then raise the nuclei to higher energy levels. When those fields are discontinued and before the nuclei return to their normal energy states, they produce radio frequency magnetic fields of their own that are detected by a spectrometer. Data is collected for a three-dimensional matrix of points, then interpreted by a computer program through image reconstruction techniques and represented visually.

The process of creating images from NMR spectroscopic data was pioneered by Dr. Paul Lauterbur, director of the UIUC Biomedical Magnetic Resonance Laboratory (BMRL). NMR imaging has been developed as a diagnostic tool capable of revealing cardiac abnormalities, hard-to-detect cancers, spinal cord injuries, kidney and liver diseases, and a host of other medical problems. Lauterbur is also refining the technique as a tool of basic research. In this research, his group makes heavy use of NCSA computational and visualization facilities and the high-speed network.

Lauterbur says, "In this work we generate huge three- and four-dimensional datasets. We require a great deal of processing to get from the original data acquisition in this laboratory to the final images. They have to be manipulated in various ways—processed, displayed, and visualized. Many researchers doing similar work have to make significant compromises, because they have limited computer power. The extensive capabilities of NCSA make it possible for us to initiate new techniques and applications."

3D NMR microscopy of a specimen of fixed human brain tissue showing fiber tracts (darkened areas). Sample is approximately 800 micrometers in diameter. Image is computed using CRAY-2 system and software developed in collaboration with NCSA. (Courtesy BMRL)



CRAY-2 in the lab

Research programmer Clint Potter, NCSA image processing specialist, has a part-time appointment in the Biomedical Magnetic Resonance Laboratory. Potter speaks of using NCSA's CRAY-2 system as a laboratory tool. "The Cray has been heavily used for simulations, but lately we've been able to bring the supercomputer into the experimental laboratory. We run an experiment and collect data on the imaging NMR spectrometer in the lab, while a process on the CRAY-2 across campus is listening, doing our image reconstruction. We're able to visualize data almost as fast as we collect it. We can get data back from the Cray in time to change the knobs on our experiments."

Lauterbur describes the impact of this advance by way of an analogy. "Anyone who has ever looked through a microscope at a specimen slide knows how you need to move the slide around to find clear features. Imagine that you had to place the slide arbitrarily, then spend a huge amount of time processing and photographing, without ever having looked through the eyepiece. Then move the slide over a fraction of a millimeter and do the same thing all over again, blindly—just seeing your data some hours or days later when the film is processed. It would be an extremely inefficient process. That is what we have had to do with NMR imaging until now. It is

---

Connection Machine (CM-2) news

by Rick Kufrin, Applications Programmer

There are two major changes to the CM-2 system at NCSA.

First is the installation of a Sun-4/490 as the new Sun front-end to the Connection Machine. Users will be happy to learn that disk space is significantly increased with this system.

Second is the installation of the 5.2 version of the Connection Machine System software. There are major changes in the graphics libraries and a newer release of the CM Fortran compiler which is available on CMVAX (CMF 0.6). In the near future, NCSA anticipates the release of a 5.2 version of the Connection Machine Scientific Subroutines Library, a set of routines that support scientific computing—especially numerical analysis. These routines are callable much like Paris routines, but they are prefixed by "CMSSL:" rather than "CM:".

Documentation covering the CMSS 5.2 release is available for viewing at the NCSA Consulting Office [see **NCSA contacts**, page 15] and also in the NCSA Numerical Laboratory, Room 3514, Beckman Institute. Users may order documentation from:

Thinking Machines Corporation
245 First Street
Cambridge, MA 02142
Attn: Order Administration

(*Adapted from the* Applications Newsletter*—monthly newsletter of NCSA Applications Group, February 1990, Melanie Loots, editor.*) ▲

Dr. Paul Lauterbur.

tremendously helpful to be able to modify experimental conditions while we're actually doing the experiment, instead of just doing it blindly."

Improved resolution

Another issue to be worked on as NMR imaging is refined involves better image resolution. Resolution is affected primarily by the diffusion of water during the data collection period. Says Potter, "We get experimental artifacts that we can't always understand."

One of Lauterbur's students, Brian Hyslop (M.D./Ph.D. [Physics] student in UIUC's Medical Scholars Program), has been simulating the effects of diffusion on microscopic NMR images and discovering some hitherto unsuspected effects.

A related collaboration with Dr. Klaus Schulten [see page 3] also involves simulating diffusion during the NMR measuring process, using the CRAY-2 system. The physical features of the simulated samples are known, so the images that result from the simulated run can be validated. Anomalies or inaccuracies in the images that result from diffusion can be investigated; the expectation is that eventually the processing codes can be enhanced to compensate for such effects.

Schulten explains, "Images are distorted through the natural process of diffusion. It not only can make things look fuzzy; in some cases, features look sharper than they really are. We have to understand how diffusion interacts with the measuring process to be capable of interpreting the images with confidence."

Commonplace miracles

When Lauterbur first thought about creating images from NMR signals, he experimented with "bits of plants, earthworms, clams, and fruit." Today Lauterbur tells his students "not to be inhibited. Don't hesitate about doing something right, for example, just because it seems to require huge amounts of computing. It may seem to *now*, but we all know how computing capabilities increase with time. What seems almost ridiculous today becomes commonplace tomorrow."

Other members of the Biomedical Magnetic Resonance Laboratory include Dr. Joan Dawson, Dr. Zhi-Pei Liang, Dr. Doug Morris, Dr. Erik Wiener, Dr. Estelle Fletcher, Howard Guenther, Carl Gregory, Sudeep Chandra, Shachar Frank, Pratik Ghosh, Haakil Lee, Alan Marumoto, Xiaohong Zhou, Patrick Moran, Brian Roman, Jyothi Raman, Joe Kmiecik, and Dipa Apte. ▲

CM-2 and visualization

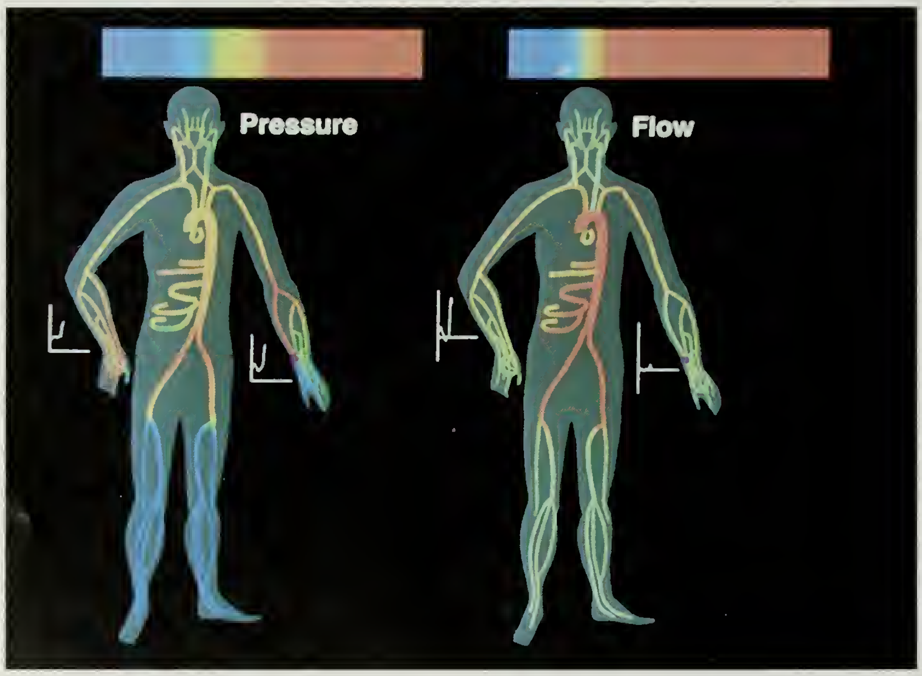
Jim Salem, Thinking Machines Corporation Scientific Visualization group leader, recently gave an NCSA-sponsored seminar entitled "The Connection Machine System and Applications in Visualization." A capacity crowd turned out to hear Salem speak at the Beckman Institute. After an introduction to the architectural and programming features of the CM-2, Salem gave an overview of its languages. This was followed by examples of visualization/graphical applications and a description of Thinking Machine's current graphics library. Videotapes of visualizations in a variety of disciplines concluded the presentation.

Cardiovascular system visualization breaks ground

by William Dwyer, Graduate Assistant Writer

As far as is known, the first animated videotape that simulates the flow of blood through a whole-body model of the human arterial system was recently produced at NCSA. It is entitled "Computer Simulation and Visualization in the Cardiovascular System."

M. E. Clark, professor in the Department of Theoretical and Applied Mechanics at UIUC, and Michael McNeill, research programmer with NCSA's Visualization Services and Development group (VSD), collaborated on a visualization project that is being well received by medical professionals and researchers in early showings.



Still from an animated sequence that shows pressure (left) and flow (right) values over the whole body's arterial system.

Using the CRAY-2 supercomputer, Clark generated data from his model of the arterial side of the cardiovascular system while McNeill created a visualization using Wavefront software on a Silicon Graphics workstation. The collaborators then made a video of animated sequences showing the *hemodynamics*, or changes in pressure and flow of blood, as it courses through the arterial system.

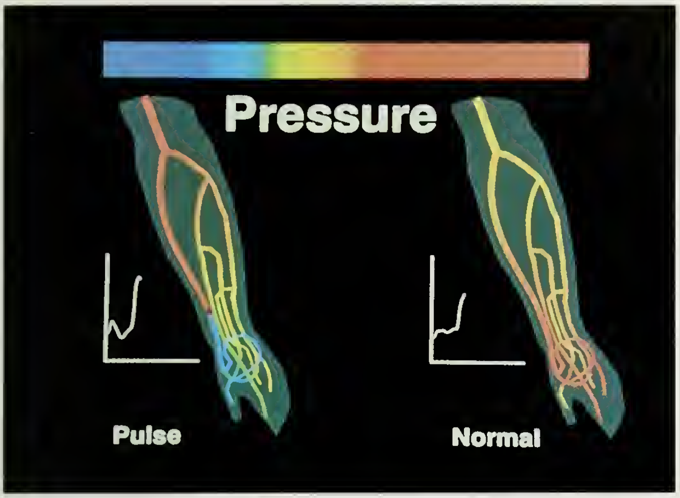
Simulating circulation over three decades

Clark, a charter member of the bioengineering faculty at UIUC, says his journey into cardiovascular system simulation began nearly 30 years ago. He developed mathematical computer models for steady pressures and flows in the circulatory system during the sixties. In the seventies with the help of Bob Kufahl, then a graduate student (now affiliated with the Louisiana State University Medical Center at Shreveport), he developed a simulation of the dynamics of cardiovascular circulation using the Navier-Stokes equations of fluid dynamics. A little over a year ago, Clark and Jan Duros, a Fulbright Scholar to UIUC from Comenius University in Czechoslovakia, used the UIUC Computing Services Office mainframe computer to do a whole-body simulation of the arterial system.

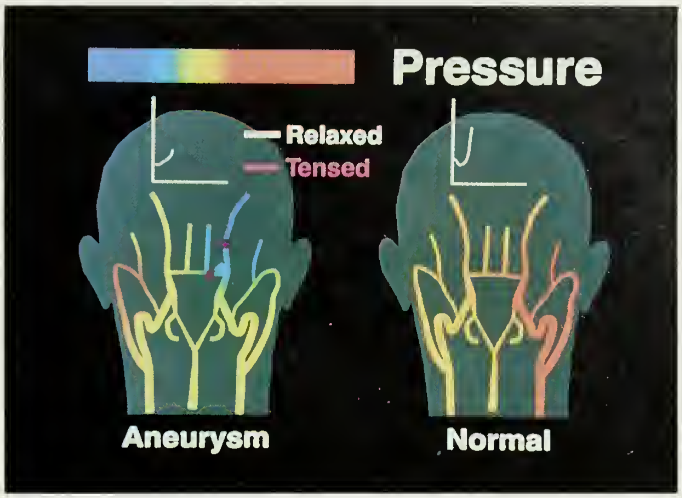
Last fall Clark was allocated time on the CRAY-2 supercomputer, and he began working with McNeill at NCSA. Clark said that after he got McNeill "straightened out about arteries and veins," they had a good time putting the video together. McNeill, after digitizing the data for the arterial pathways, took the data for vessel size and used the Duct software program developed by Jeffery Yost, former scientific animator at NCSA now working in Germany, to get a smooth-tube representation of the arteries.

Using NCSA Image software from the NCSA Scientific Visualization Software Suite [see ***access***, July–August 1989], McNeill manipulated colors on a palette to get a broad color spectrum that shows where major changes in data occurred. McNeill said the project was an interactive situation. As the visualization work progressed, viewing the data in this new format generated the desire to observe the effects of changing other parameters as well. This project could serve as an example of

Comparison of pressure values in the left arm between taking the pulse (left) and normal (right) cases.



Comparison of what happens when an aneurysm is present (left) in the blood circulation of the brain with normal circulation (right).



the central purpose of scientific visualization.

Prior to his work with NCSA, Clark says he was limited to simulating blood flow in separate areas of the cardiovascular system. These models did not allow for the inherent interaction of various areas. NCSA's equipment and McNeill's expertise enabled the bioengineer to simulate and visualize blood flowing through all parts of the body's arterial system *simultaneously*—much as in reality. According to Clark, this aspect of the videotape makes it unique.

Using 120 frames per heart period, the video develops an understanding of the dynamic action and interaction of various components of the arterial system in three steady-state situations and one transient episode. Two human silhouettes are shown. One represents pressure changes; the other, changes in blood flow. Red hues are used for high pressure and flow; blue hues for low pressure and flow in the 96 "judiciously selected" simulated vessels. Graphs, depicted like those shown on EKG monitors, track alterations of pressure and flow with time at selected sites in the model.

A final sequence charts what happens in the human brain when an aneurysm is present in the cerebral circulation. Comparative views of normal blood circulation appear beside those simulating the aneurysm. In this pathological simulation, Clark noticed several phenomena that have yet to be explained. Asymmetry of blood flow from the heart caused by the manner in which the various arteries branch from the aortic arch reproduces asymmetric circulation throughout the upper part of the body. This observation clearly shows in the aneurysm sequence. "When I first looked at the results on the video," Clark states, "I could hardly take in all I was seeing."

Getting positive feedback

People who have seen this visualization of the first known whole-body view of changes in the circulatory system are enthusiastic. Its premier public showing took place in December 1989 before physicians of the Champaign County (Illinois) Medical Society who attended the Supercomputing in Medicine Seminar at the Beckman Institute. Clark's video was part of his keynote address, "A Supercomputing Look at the Cardiovascular System."

Dr. Frank Wrestler, director of MEDnet, organized the seminar. The UIC College of Medicine at Urbana-Champaign, MEDnet, NCSA, and the medical society were cosponsors together with the UIUC Department of Health and Safety Studies and McKinley Health Center. According to Wrestler, medical doctors—who are not very well trained to view physiological phenomena as data that can be quantified, modeled, and predicted—were "extremely favorable and laudatory" toward Clark's presentation. Wrestler has asked Clark to give a presentation to the medical staff at UIUC's McKinley Health Center. Also Wrestler thinks there might be considerable interest among the medical school classes and resident staffs at the UIUC and UIC campuses.

Clark sent a copy of the videotape to a recognized authority in the field of bioengineering, Dr. Y. C. Fung, professor of bioengineering at the University of California at San Diego. Fung said that he watched the video for hours and wrote to Clark: "What a delight in watching those pressure and flow traces animated with color code of the whole man!"

The video has been accepted for showing at the First World Congress of Biomechanics, August 30–September 4, 1990 in La Jolla, CA. Clark plans on using the video for other upcoming presentations.

Partial funding for the production came from the UIUC Research Board and Erdman Associates, Haverstown, PA. NCSA postproduction work was done by Bob Patterson, production manager, and Cordelia Baron, media production specialist, of NCSA Media Services. ▲

Towards a distributed visualization environment

by Jarrett Cohen, Public Information Specialist

The 1950s saw the arrival of the computer and with it a new method of inquiry—computational science. Particularly with high-performance computers and three-dimensional graphics, computational science has allowed researchers to understand previously unseen phenomena.

NCSA has refined a team production visualization approach, the end result of which are high-quality videotapes. The Visualization Services and Development group (VSD), managed by Dan Brady, has won numerous awards for its efforts [see ***access***, January 1990].

This team approach continues to be an important method for research into new data visualization models. To extend its success, VSD has embarked on new initiatives that center on delivering visualization productivity to the general user community. One of these initiatives has the goal of refining interactive visualization techniques to the same extent as the group's videotapes.

Combining technologies

NCSA has been involved in the development of distributed visualization for several years. This approach centers on the concept of graphics workstations networked to supercomputers. It allows data computed on a supercomputer to be graphically processed on a workstation. The ideal is to have the computation and graphics occur in real time.

To explore distributed visualization, a CRAY-2S/4-128 supercomputer has been combined with a Silicon Graphics IRIS 4D/240GTX workstation and existing Ethernet networks. The NCSA CRAY-2 provides typical single processor speeds of 100 Mflops sustained in addition to its large, fast memory and disk capacities. SGI's IRIS adds the graphics rendering power of 100,000 shaded polygons/sec with hidden surfaces removed.

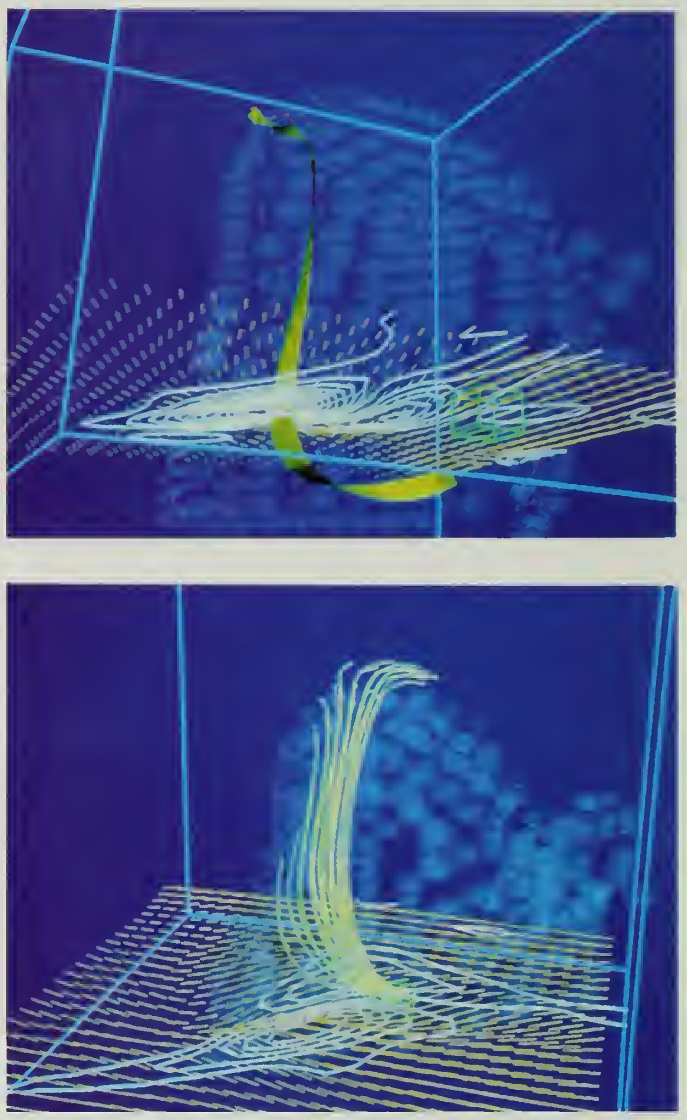
SGI's Distributed Graphics Library (DGL) product makes this combination possible by allowing graphics commands to be sent from the CRAY-2 system to the SGI workstation over Ethernet in real time.

NCSA is developing from this system platform an advanced computing model in the VSD Numerical Laboratory Visualization Project. Ray Idaszak, VSD Numerical Laboratory project leader, is supervising the construction of a methodology that extends into the realm of true heterogeneous multicomputing. In this environment, all computational resources are accessible from high-speed graphics workstations.

Interactive storm simulation

To test this new, distributed system, Idaszak; Lou Wicker, graduate research assistant in meteorology; Crystal Shaw, research programmer; and Bob Wilhelmson, NCSA research scientist and UIUC professor of meteorology, implemented a numerical storm simulation in real time.

The software environment used to create the model includes DGL, the NASA Panel Library, and in-house visualization and simulation code.



Two views of a transparently represented thunderstorm using contours, vectors, and twisting ribbons from an interactive distributed visualization between a Cray-2 supercomputer and a Silicon Graphics workstation. (Credit: Bob Wilhelmson, Lou Wicker, Crystal Shaw, and Ray Idaszak of NCSA)

"Our initial goal was to come close to visually reproducing the videotape 'Study of a Numerically Modeled Storm' in real time in a distributed environment," said Idaszak.

"The resulting interactive visualization has much of the same informational content as the video" said Wilhelmson. "The interactive software incorporates many of the same visual idioms as the video, although interactivity is accomplished at the expense of the quality of the visual presentation."

Wicker pointed out that "distributed interactive visualization has several advantages. It allows the scientist to

Towards *continued on page 14*

STG releases NCSA ImageIP

by Jill Peacock, Editorial Assistant, Software Tools Group

Last month the NCSA Software Tools Group (STG) released the first version of NCSA ImageIP (Image Processing), a color image analysis program. Funded by money from Apple Computer Inc. to MEDnet (Medical Network), the program was created to analyze and manipulate images.

MEDnet is an innovative, multidisciplinary program for health care professionals that focuses NCSA's advanced computational resources on a range of health care problems [see ***access***, January–February 1989]. The program is supported by several departments at UIC and UIUC, McKinley Health Center, and the Champaign County (Illinois) Medical Society. Dr. Frank A. Wrestler, staff physician at UIUC's McKinley Health Center, is its director.

Applications of the program

The medical field is one of many possible areas for the application of NCSA ImageIP. Specifically ImageIP can be used to analyze computed tomograms, x-ray photographs taken of a single plane in which structures in other planes are eliminated; magnetic resonance imaging (MRI) images, images that are obtained using a varying magnetic field and subjected to a pulse of radio frequency magnetic fields which produce spectra that are combined into cross-sectional images; and other forms of medical and nonmedical images.

According to scientific programmer Mark Stupar, one of the main contributors to the software's development, the NCSA ImageIP program enables users to perform important data analysis and scientific visualization at a local desktop workstation. Unique to NCSA ImageIP is the ability to actually change the displayed data for intensive investigation. Based on NCSA Image [see ***access***, March–April 1989] which simply displays data, ImageIP was further developed to alter data.

Dr. David Lawrance, assistant director of MEDnet and assistant professor of internal medicine at UIC's College of Medicine at Urbana-Champaign and NCSA, explains the advantage of software that enables medical image processing. Once an image has been derived, from either healthy or abnormal tissue and cells, "these programs allow greater analysis since you can examine 2D slices of the image and then put them back into a 3D volume." With traditional analysis tools, such as x-ray machines, "you only have one shot at a 3D image, so you miss a lot of things." According to Lawrance, another problem with x-rays and CAT scans is that they use "ionizing radiation versus MRI which uses radio frequency magnetic fields to get structural images." Thus, programs that can analyze MRI images offer more options to medical specialists.

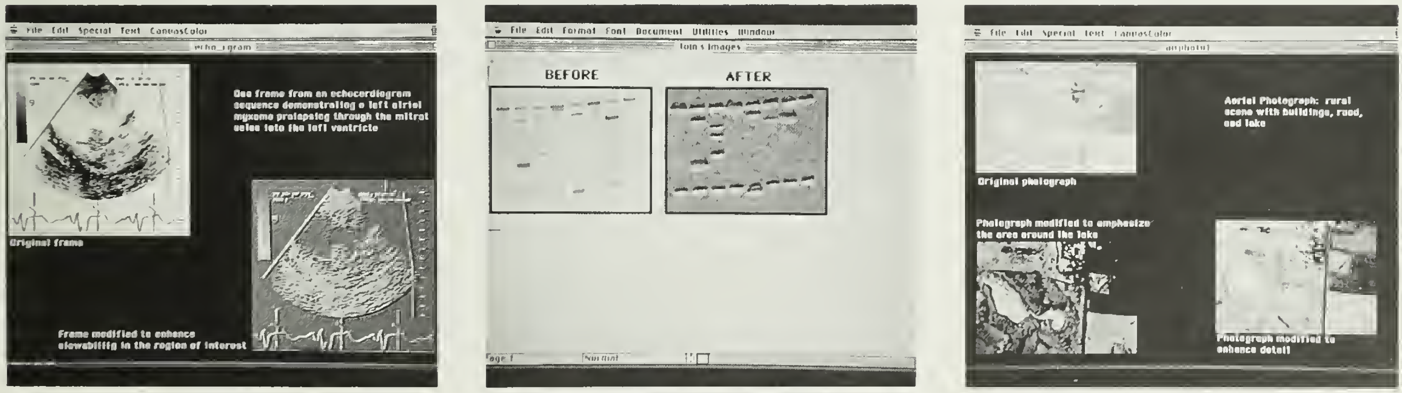
General uses of the program

NCSA ImageIP application also broadly extends outside the medical establishment. Stupar foresees the program being used in satellite imaging (for terrain pictures) and also as a photo-enhancer, since NCSA ImageIP can clear up grainy images. Lawrance agrees that imaging programs have become valuable in retouching photographs.

Molecular biologists, for example, will be able to improve the quality of their scanned, digitized electrophoretic gel images. Using NCSA ImageIP, they can reduce background noise as well as smooth and enhance contrast in images, thereby improving the quality of the analysis of their gels.

Clint Potter is a research programmer who, over the past two years at NCSA, has worked on collaborative NMR

***STG** continued on page 13*


File Edit Special Text CanvasColor
echo_gram
One frame from an echocardiogram sequence demonstrating a left atrial myxoma prolapsing through the mitral valve into the left ventricle
Original frame
Frame modified to enhance viewability in the region of interest
File Edit Format Font Document Utilities Window
Tom's Images
BEFORE
AFTER
File Edit Special Text CanvasColor
Aerial Photograph: rural scene with buildings, road, and lake
Original photograph
Photograph modified to emphasize the area around the lake
Photograph modified to enhance detail

Before and after views show how NCSA ImageIP software can improve images in many disciplines. In medicine (left), an echocardiogram sequence enhanced with modifications; in molecular biology (center), an electrophoretic gel with reduced background noise and smoothed and enhanced contrasts; and in aerial photography (right), a topological view with enhanced landscape details. (Courtesy STG)

Center cache

by Fran Bond, Technical Editor

Several personnel changes were recently announced at NCSA. New positions, promotions, and appointments are as follows:

Donna Cox is now associate director for Education. In this newly created position, Cox provides leadership in facilitating, coordinating, scheduling, and approving educational and training activities in the Renaissance Experimental Laboratory of the NCSA Numerical Laboratory located at the Beckman Institute. She also plays an important role in facilitating and coordinating all other activities in the Numerical Laboratory, such as providing access and help for the user community. Within NCSA, she acts as an advocate for users' needs in relation to the Numerical Laboratory. As associate director for Education, Cox reports to Karl-Heinz Winkler, deputy director for Science, Technology, and Education (STE). Prior to this appointment, Cox was an NCSA design and research professor; she continues as a UIUC associate professor of art and design. She has a two-thirds time appointment with the School of Art and Design, and one-third with NCSA.

In mid-February, **David Curtis** assumed the duties of associate director for Information and Publications. In this position, he is overseeing the Publications Group and the Public Information Office. Curtis recently arrived at NCSA from New York City where, since 1983, he produced and directed science programming at WNET/13, one of the leading PBS stations in the country. His credits include "Innovation," the nationally distributed Emmy award-winning science documentary series. Also, for the last five years, Curtis has worked on a number of independent educational and documentary projects for several major clients such as AT&T. Employing his television experience and aided by a strong science background, including a Ph.D. in biochemistry, Curtis plans to strengthen the public visibility of NCSA through a variety of media—particularly video. He will report to Jim Bottum, deputy director for Operations, Planning, and Client Relations (OPCR).

Virginia Hudak-David has accepted the position of assistant director for Administrative Affairs in the Department of Finance and Administration. In this new position, she is responsible for administration, human resources, and reporting/proposal development. She reports to Deborah Lee, associate director of Finance and Administration, and directly manages Administrative Services, Human Resources, and Institutional Information. Formerly Hudak-David was staff associate to OPCR deputy director, Jim Bottum.

Recently **Sandra Long** was promoted to assistant director of Business Affairs. Business Affairs provides business and financial services to NCSA, including procurement, reimbursement, reporting, grant administration, proposal budget assistance, shipping, receiving, travel, inventory, and other related tasks. Prior to her promotion, Long was acting assistant director of Business Affairs. In this new position, Long reports directly to Deborah Lee, associate director of Finance and Administration.

Marcia Miller was appointed assistant deputy director for Science, Technology, and Education (STE). In her new position, Miller is responsible for administering day-to-day operations and internal affairs of the office of Karl-Heinz Winkler, STE deputy director, and acts as Winkler's representative in discussions. She also serves as administrative liaison to the associate directors in STE and OPCR. Before assuming these duties, Miller was manager of Human Resources and acting manager of Administrative Services.

Nora Sabelli is assistant director of Educational Outreach in the Academic Program. She is responsible for developing NCSA's discussion, dissemination, and evaluation of the uses of high-performance computing in science and technology education for precollege, college, and teacher education faculty and students. In addition she is working with other educationally oriented groups that lack working access to high-performance computing resources or are interested in adapting NCSA's strategies for high-performance computing in education. Sabelli participated in the High Performance Computing and Networking for Science Advisory Panel of the Office of Technology Assessment. Through this and other committees, she is engaged in computational science at the national level. She continues her duties as NCSA senior research scientist and associate professor in the UIC Department of Chemistry. In this new appointment, Sabelli reports to Scott Lathrop, associate director of the Academic Program. ▲

Bottum gets you to the top

by Kathleen Robinson, Science Writer

Jim Bottum, Deputy Director.

In February, NCSA users received letters announcing yet another title for OPCR Deputy Director Jim Bottum—that of ombudsman for researchers using the center. “Recognizing that NCSA is getting bigger and more complicated organizationally, we wanted a way for any researcher, institution, corporation—anyone affiliated with NCSA—to resolve problems, to go straight to the top if need be,” says Bottum.

The term ombudsman surfaced shortly after Bottum came to the center in 1986 as visiting assistant director on sabbatical from the NSF. “One of our users who was then at Cal Tech, John Hawley, said he liked having an advocate, an ombudsman, within the organization. I’ve been a troubleshooter for users on an informal basis since I first came, but with the structural reorganization that NCSA underwent late last year, the Director thought it was time to make the role official.”

One of the goals of the 1989 reorganization that Bottum referred to and that brought STE Deputy Director Karl-Heinz Winkler to the center was to separate user representation from the technical side of NCSA and to create a channeling function for information between the two. With this structure in place, the technical staff concentrates on providing service and enhancing that service for users. The Academic and Industrial Programs have staff members whose jobs are to keep their fingers on the pulse of NCSA’s user community.

Reacting to the suggestion that he may find himself even busier than before, Bottum says, “If that’s what happens, that’s good—that’s what I’m here for. There is nothing more important that I could be working on. NCSA exists to serve its users. I should point out though that I am a last resort for someone who is having a problem. There are teams of problem solvers throughout the center for users to consult. My presence as ombudsman should be viewed as insurance. When someone is really having a problem that’s not being addressed, that’s when I go into action. I view my most important job as representing users of the center.” ▲

Training & Education

Affiliates Program grows

by Scott Lathrop, Associate Director, Academic Program

The NCSA Affiliates Program is composed of both the Academic Affiliates and the Scientific Institute Affiliates that now total more than 90 institutions.

The Academic Affiliates Program has gone through a number of staff changes since its inception by Joseph Hardin, now manager of the Software Tools Group. Most recently, Janice Knapp-Cordes has been the acting coordinator. We are very pleased to announce that Dave McWilliams has been appointed academic affiliate coordinator.

McWilliams began his employment at NCSA in 1986 as a systems consultant and became the manager of Consulting during 1988. Until recently he managed the Systems Integration Group which was focused on UNIX software development efforts. McWilliams brings to the academic affiliate coordinator position considerable expertise with NCSA’s systems as well as a history of support and concern for its clientele.

The Academic Affiliates Program is open to any academic institution that wants to provide a local high-performance computing support infrastructure to its institution. An affiliate representative receives training at NCSA, a block grant of time on the CRAY X-MP system to allocate to researchers and classes for startup and experimentation purposes, and technical documentation and support.

Dr. Barbara Mihalas, formerly a member of the Research Scientist group, has been appointed the scientific institute affiliate coordinator. She will assist scientific institutions in forming joint collaborations with NCSA for research and for software and technological development.

Mihalas’ research is in the areas of radiation-hydrodynamics, waves and oscillations, and radiative transfer. She is involved with a large research effort investigating helioseismology and stellar seismology. She has also done research in scientific data management and is principal investigator of an NSF grant for further research in that area. Since 1985 she has been a research scientist at NCSA; she is an adjunct assistant professor in the UIUC Department of Astronomy.

Please give McWilliams or Mihalas [see **NCSA contacts,** page 15] a call if they can assist you in any way. ▲

Announcing the NCSA Academic Program

by Scott Lathrop, Associate Director, Academic Program

The Academic Program was recently formed to focus attention on the needs of the academic community. The Academic Program combines the talents of the following people and groups:

Client administration—Patricia Wenzel and her staff—Judy Olson, Jody Francis, and Cindy Maxey—can assist you with any questions or problems related to accounts, signons, the peer review process, and visits to NCSA. The Visitors Program provides working space and facilities to support researchers who would like to spend time at NCSA to focus on their work and to interact with the NCSA staff, partners, and UIUC faculty.

Training and outreach—NCSA provides technical classes on the use of high-performance computing tools and facilities through sessions at NCSA as well as at remote sites. Lyle Rigdon and his staff, Janice Knapp-Cordes and Karen Gobble, can provide information on technical training events. They will assist you with registration and are eager to hear from you about how training classes could be altered or modified to meet your needs. Rigdon can work with you to arrange outreach training events at your site as well.

Educational outreach—Dr. Nora Sabelli works with educators at all levels (precollege to professional) to develop materials and strategies that incorporate computational science into curricula. The Educational Outreach Program provides grants of supercomputer time to support regular classes and course projects.

National client program—The national client program is an outreach to the community to ascertain its needs and to help provide support at local sites. The program has two components: the Academic Affiliates Program and the Scientific Institute Affiliates Program.

1. The Academic Affiliates Program provides local support for researchers on their own campuses through the local affiliate representatives. Dave McWilliams is available to work with affiliate institutions and representatives to provide training, support, and a voice into NCSA. This program is also intended to help local researchers get startup grants to explore the use of supercomputing and develop requests for larger grants of time.

2. The Scientific Institute Affiliates Program is a new program that expands our affiliations to scientific institutions. Dr. Barbara Mihalas is available to establish extended communications between NCSA and institute staff and researchers. Scientific affiliates receive support like NCSA's academic affiliates. This affiliation is based on a mutual expectation of developing collaborations between the scientific institutes and NCSA in areas such as software development, workshops, and research projects. The objective is to combine the talents and resources of NCSA and its affiliates to further their goals. Kendra Reasor supports the Affiliates Program and can help you get answers to your questions.

Throughout the year, we will be surveying the research community to learn how we might further improve the services and facilities at NCSA. We are always interested in hearing from you—we appreciate your comments, criticisms, and suggestions for ways that NCSA can better enable you to accomplish your objectives.

Please feel free to contact me, or any other member of the NCSA staff [see **NCSA contacts**, page 15], to let us know how we might better serve you. ▲

Upcoming NCSA workshops/conferences

Finite Element Conference May 14–15
For more information, contact Ilhan Dilber, industrial consultant, at (217) 244-1973 or idilber@ncsa.uiuc.edu (Internet); 13024@ncsavms (BITNET).

Molecular Modeling Workshop June 11–15
For more information, contact Nora Sabelli, senior research scientist, at (217) 244-0644 or nsabelli@ncsa.uiuc.edu (Internet); 10241@ncsavms (BITNET).

Networking and Supercomputing Conference (date to be announced)
For more information, contact Charlie Catlett, manager of Networking, at (217) 333-1163 or network@ncsa.uiuc.edu (Internet); network@ncsavms (BITNET).

Note: Announcements with details of these workshops/conferences will be sent to all users. If you are not on the NCSA newsletter mailing list, contact the appropriate individual above to receive an announcement.

New and updated online information

by Will Ridenour, Online Documentation Editor

The following help files, documents, and man pages have been added or updated as of February 5, 1990.

UNICOS help files

Name	**Description**
catalog	*The NCSA* Technical Resources Catalog
contacts	*Whom to contact for various problems*
affiliates	NCSA affiliate contacts
software	*The latest list of software on NCSA machines*
training	*Information about NCSA user training*

To access a help topic, enter: **`help topic`**
where *topic* is the name of the topic you wish to view.

UNICOS documents

Name	**Description**
index	*Indexes for NCSA newsletters*
access.89	Index for 1989 ***access*** issues
datalink.89	Index for 1989 ***data link*** issues
lapack	*Documentation for the lapack linear algebra package*
complex	Complex routines
single.precis	Single-precision routines
online.list	*The latest list of NCSA online documentation*

To access an online document, change directories to /usr/local/doc and enter: **`more docname`**
where *docname* is the name of the document you wish to view.

UNICOS man pages

Name	**Description**
specfun	*A library of special function software*
spssx	*Comprehensive statistical package*

To access a UNICOS man page, enter: **`man manpage`**
where *manpage* is the name of the man page you wish to view.

STG *continued from page 9*

(nuclear magnetic resonance) imaging microscopy projects with Paul Lauterbur [see page 4]. Before coming to NCSA, Potter worked on remote sensing at ITEC Optical Systems and prior to that at the Children's Hospital in Boston on radionuclide imaging.

Potter sees the software program as a big advantage to computational scientists who are now performing simulations with NCSA Image. He says, "It wouldn't take them long to figure out that some of the contrast enhancement techniques in NCSA ImageIP might be useful in the analysis of simulation data." He adds that "because NCSA ImageIP is free, it will hopefully allow people unfamiliar with imaging techniques and those in that field to begin experimenting with no risk. The program incorporates some basic image enhancement techniques into the NCSA Scientific Visualization Software Suite."

NCSA ImageIP features

Features of NCSA ImageIP Version 1.0 for the Macintosh allow you to do the following:

- use color, contour plots, 3D plots, shaded data plots, XY plots, and ordered dither plots to display sets of data points
- select imaging and analysis tools, or mouse action modes, from a special tool chest
- copy to the Clipboard and paste into other applications color raster images, palettes, and black-and-white plots
- print contour, shaded data, 3D, and ordered dither plots, as well as XY graphs
- modify and save color palettes
- animate and magnify multiple raster images
- display rulers in the image window
- animate sequential raster images
- enable use of contrast modification utility
- specify filters and convolution kernels
- display histogram equalizations and specifications
- record operation history

To obtain a copy

To order a copy of NCSA software, refer to the March NCSA *Technical Resources Catalog*.

Future versions of ImageIP

Future versions of NCSA ImageIP will include more analytical functions. Frequency-domain analysis, a more complex analytical tool, will be used. Stupar says the new tools will be aimed toward helping users identify information within the image.

Biological *continued from page 3*

seen in experiments on the monkeys. Now we feel we can understand an important step in the self-organization of neural tissue—namely, the capacity of neural tissue to find its own connections while the neural systems are being used."

Baby robots

Neural research led Schulten to work on an even more complex level of biological organization. Says he, "The most impressive capacity of neural systems is not that they *receive* information, but that they can process it and act accordingly." To test the ways in which neural self-organization may influence learning, Schulten simulates very complex robots on a Silicon Graphics 220 GTX workstation. "Until now," he says, "robots were programmed to do repetitive tasks." Schulten's simulated robots can learn to move and adjust their motions to changes in the environment—a logical advance in their evolution. Members of the group working on this project are Thomas Martinetz, Joerg Walter, and Benno Nieswand.

"We simulate an extremity like a complex arm with many muscles, then we put stereo cameras between the arm and the brain of the robot," Schulten explains. "The brain receives the camera output and is connected to the lines that feed the motor signals to the arm, to move it. Using some very simple rules, this system can organize itself to move the arm correctly. It behaves very much like a baby. Initially it can make only simple, inaccurate motions. And with time—now we are speaking of a matter of minutes—while we watch the robot perform on the computer, it actually learns to move better. After about 10 minutes, the robot arm can move very accurately and grab objects. Of course we need pretty impressive computer power behind that." Schulten was recently awarded funding from the State of Illinois through the Beckman Institute to build hardware versions of some of these self-taught robots.

Schulten believes his team has discovered an important principle that may explain why the brain has such great capacity. "We think the brain tries to spatially order its tasks so that similar tasks are being performed by neurons that are very close together, while tasks that are less similar are taken care of by neurons that are farther apart. This principle of spatial relationship—called *topographic order*—allows the neurons to cooperate while they learn. If one neuron performs its task better, that capacity can be copied by neighboring neurons which are responsible for similar tasks. As a result, relatively few training instances are needed to train an entire network."

Broad expertise

Others in the Theoretical Biophysics Group are Andreas Windemuth and Bernard Walberer, who work on protein folding; Christian Kurrer, who studies theoretical high-temperature superconductivity and nonlinear dynamic systems; and Markus Van Almsick, who investigates quantum logic and is an expert with the program *Mathematica.*

Summing up the relationship between his group and NCSA, Schulten says, "We feel this kind of work is very well supported by NCSA—not only in the computing component, but because NCSA brings together scientists and experts from very disparate disciplines. This lodging of computational expertise and of scientific interest spills over to the users and helps them in many ways." ▲

Training dates: 1990

April 23–27	New User Training	June 4–8	New User Training
May 19–20	MEDnet Training	July 23–27	New User Training
May 21–25	New User Training	August 20–24	New User Training

Note: Dates are subject to change. Class size is limited. You must register to attend NCSA training.
To register: Academic users contact Karen Gobble at (217) 244-4198. Industrial partner users contact your representative at NCSA.
For additional information: Contact Lyle Rigdon at (217) 244-3659 or at lrigdon@ncsa.uiuc.edu (Internet) or 815@ncsavms (BITNET).

Towards *continued from page 8*

combine computational resources in such a way as to enable efficient interrogation of one's data." Just as in the 1980s when NCSA provided its users with the ability to do remote interactive supercomputing, NCSA in the 1990s hopes to lead the way in making interactive distributed visualization available to its users.

A model for the 1990s

This distributed environment, which will become commonplace in the 1990s, can only be fully taken advantage of with further advances in gigabit networking technologies. For today's workstations, approximately 10 to 14 Mbytes/sec sustained *per user* are needed. NCSA, SGI, and others will continue their efforts to influence Congress and vendors to make this performance available on a national scale. ▲

NCSA contacts

General information and machine access

NCSA Receptionist
(217) 244-0072
FAX (217) 244-1987

Orders for Documentation and Publications
Debbie Price
(217) 244-4130

Cray Operations
(217) 244-0710

Dialup Access—2400 baud or less
(217) 244-0662

Dialup Access—9600 baud
(217) 244-6733

CM Sun front-end address
cmsun.ncsa.uiuc.edu (128.174.220.4)

CM VAX front-end
cmvax.ncsa.uiuc.edu (128.174.220.5)

CRAY X-MP IP address
ux.ncsa.uiuc.edu (128.174.10.46)

CRAY-2 IP address
u2.ncsa.uiuc.edu (128.174.10.44)

ULTRIX gateway addresses
ncsagate.ncsa.uiuc.edu
(128.174.121.38) (Internet)
ncsagate (BITNET)

Anonymous FTP IP address
ftp.ncsa.uiuc.edu (128.174.20.50)

NSFNET Problems
(617) 873-3400

NSF Network Service Center
nnsc@nnsc.nsf.net

SRI-Network Information Center
(415) 859-3695
nic.ddn.mil

Programs and mailing lists

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uadmin@ncsavms (BITNET)
uadmin@ncsaa.ncsa.uiuc.edu (Internet)

Thanks for your help

by Fran Bond, Technical Editor

NCSA thanks the following principal investigators who cooperated with writer William J. Kaufmann III to produce the award-winning brochure, *Science Highlights 1988: Creating New Advances in Computational Science.*

In order of appearance
David Onstad, Illinois Natural History Survey
"The European Corn Borer"

J. Andrew McCammon, University of Houston
"Molecular Design"

Charles R. Evans, California Institute of Technology
"Colliding Neutron Stars"

Robert Wilhelmson, NCSA and UIUC
"Severe Thunderstorms"

John F. Hawley, University of Virginia; and
Omer M. Blaes, California Institute of Technology
"Disk Instabilities around Black Holes"

Bruce Berne, Columbia University
"Disordered Many-Body Systems"

R. Stephen Berry, University of Chicago
"Melting and Freezing of Microclusters"

Henry Krakauer, College of William and Mary
"High-Temperature Superconductors"

Michael Norman, NCSA and UIUC; and **Jack Burns** and **Martin Sulkanen**, University of New Mexico
"Disrupted Jets from Active Galaxies"

Mark Ratner and **Donald Ellis**, Northwestern University; and **Paul D. Hale**, Brookhaven National Laboratory
"Building Molecular Metals"

Robert Haber, **Hyun Koh**, and **Hae-Sung Lee**
NCSA and UIUC
"Crack Propagation"

The brochure was entered for competition in the 17th Annual Technical Communications Awards Program sponsored by the Chicago Chapter of the Society for Technical Communication (STC). At STC's annual awards program (in December 1989), *Science Highlights 1988* won two awards: Excellence for Design Graphics—Brochures in the Art Awards Section and Merit for Promotional Materials in the Publication Awards Section. In May, the brochure will compete in the 37th International Technical Communications Conference at Santa Clara, CA.

Virginia Worthington designed the brochure; Colleen Bushell and Stefen Fangmeier were art director/illustrator and technical director respectively for cover artwork. The cover featured a cubistic collage of stills of various NCSA-produced visualizations and related visual images produced at the center [see ***access***, January 1990]. Others involved in producing the brochure were Fran Bond, editor/coordinator; Melissa Johnson, managing editor; and Mary Hoffman and Kathleen Robinson, assistant editors. ▲

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- New man options make finding information easier
  by Will Ridenour
- SLADOC facility available on the NCSA Cray systems
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- SPECFUN available on the NCSA Cray systems
  by Beth Richardson
- SPSSX available on the NCSA CRAY-2 SYSTEM
  by Beth Richardson

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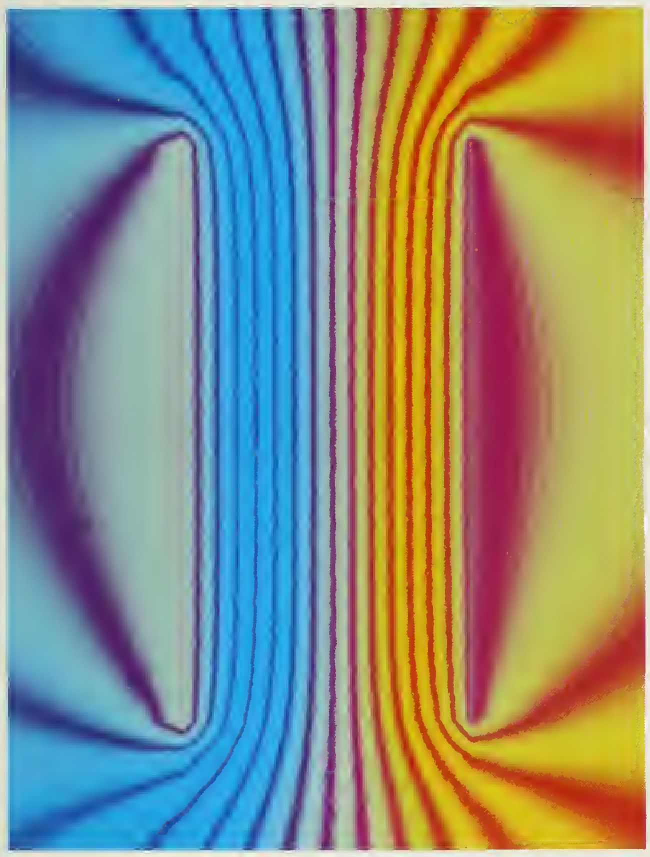

Numerical solution of Laplace's equation showing the equipotential lines of an electric field generated by charged parallel plates. Both this image and the image on page 3 are frames from a video produced by David Renneke using NCSA-developed software in the public domain.

Affiliates

Introducing undergraduates to high-performance computing

by Randall Graham, Science Writer

Today's aspiring scientists must know more than their science; they must also be skilled with supercomputers. High-performance computers are becoming the central tools of science—not only in research, but also in day-to-day applications such as design, prototype simulation, and testing. The ability to visualize numeric data with animated supercomputer models is making the invisible visible, the unintelligible understandable, the impossible possible.

David Renneke, Augustana College physics professor and chair of the division of natural sciences, is introducing his undergraduate physics students to supercomputing using a toll-free telephone line and the CRAY X-MP/48 system at NCSA. Augustana College in Rock Island, IL, is one of the center's newer academic affiliates, having joined the program last summer [see ***access***, July–August 1989].

In this new course, Renneke's students first conduct a lab experiment designed to map and measure electric fields described by Laplace's equation. Then they solve the mathematical equivalent on three different computers—an IBM PC AT with a math coprocessor, a MicroVAX II, and the CRAY X-MP system. This enables the students to compare the speeds of the various computers as well as their accuracy with respect to the observed data. Renneke says the differences are dramatic. "The IBM PC AT took approximately 280 times longer than the Cray. The numerical results were all within a few percent of the lab data."

Developing the syllabus

Renneke developed the outline for his undergraduate course at NCSA's Summer Workshop on Supercomputing Education in July 1989, conducted by Dr. Nora Sabelli, a

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page 4	Photo by NCSA Media Services.
page 6	Photo by BIMA.
page 7 left	Visualization by BIMA; image produced on NCSA CRAY-2 system. Continuum data from VLA observations by K. Y. Lo; HCN molecular data from BIMA observations by M. C. H. Wright.
page 7 right	Visualization by BIMA from image generated with MIRIAD software on NCSA CRAY-2 system.
page 8	Visualization by Donna Cox on a Silicon Graphics IRIS using Wavefront Technologies software.
page 9	Visualizations by Ray Idaszak and Donna Cox on Alliant FX/8 using Wavefront Technologies software.
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Abbreviations

CRI	Cray Research Inc.
DARPA	Defense Advanced Research Project Agency
IRP	Interdisciplinary Research Program of NCSA
NCAR	National Center for Atmospheric Research
NCSA	National Center for Supercomputing Applications
NSF	National Science Foundation
UIC	University of Illinois at Chicago
UIUC	University of Illinois at Urbana-Champaign

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Undergraduates continued from page 1

scientist working at NCSA to develop educational outreach programs. It was there that he first used the Cray supercomputer to solve the electric field problem now being tackled by his students.

While at the workshop, Renneke discovered that he could use NCSA-developed public domain software for the Macintosh to easily produce on videotape an animated color visualization of the experiment. Renneke explains how: "I considered modifying the Fortran program to write the results out in HDF (Hierarchical Data Format), but time was limited so I wrote the solution matrix to an ASCII text file. I included the appropriate header lines so that the file could be read by the Macintosh program NCSA DataScope via the text window. This worked very well. After examining the results graphically, magnifying, and adding an appropriate color palette, I saved it as an HDF file. Then I switched to NCSA Image, read the HDF file, and used the palette rotation tool to illustrate the physics of the model—in particular, the manner in which an electron would move when placed in the electric field between and around the plates. This pseudoanimation via cycling the color palette was very effective."

Renneke had found more excitement to share with his students. "An animation really enhances the student's understanding of the phenomenon taking place," said Renneke. "NCSA's software is so user friendly, you can easily learn how to use it and quickly apply your own creativity to initiate results."

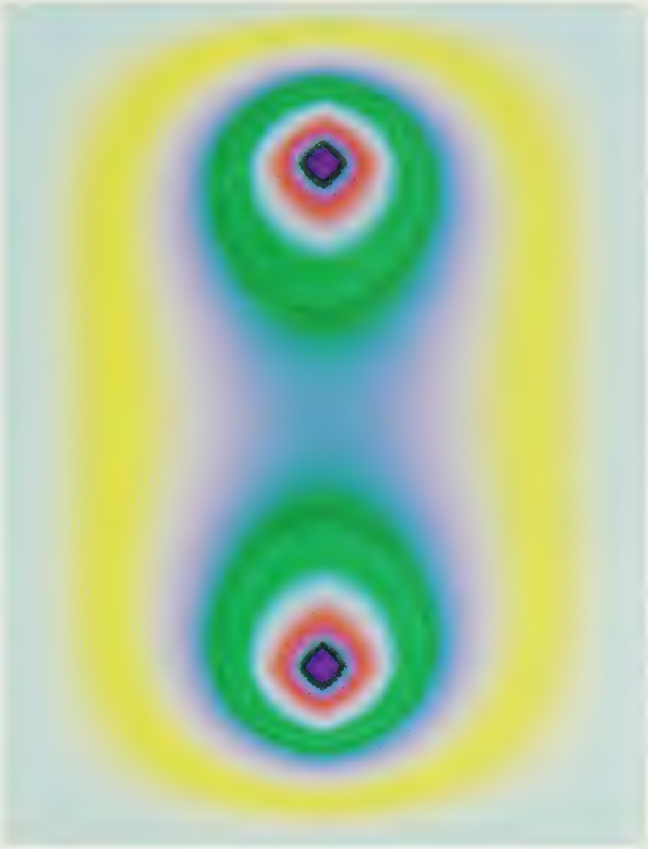
NCSA programs bear fruit

Renneke's enthusiastic response to the workshop is a perfect example of what NCSA is accomplishing through its educational outreach and academic affiliates programs. He not only teaches students how to use the supercomputer and its related facilities, but he is igniting interest among other educators as well. For example, at the fall 1989 meeting of the Illinois section of the American Association of Physics Teachers, Renneke's 20-minute talk included his experiences with NCSA.

The 91 institutions in NCSA's Academic Affiliates Program include undergraduate institutions and a high school, testimony to the center's strong commitment to making the tools of computational science available to a large and diverse community of users. Emphasis in the coming year will be on strengthening the affiliation with each institution to help remote users get the most out of NCSA.

Renneke's enthusiasm for supercomputing has prompted him to ask NSF to help fund an upgrade of computer facilities at Augustana College that would include five Sun Workstations and a network connection to NCSA. Sabelli has written NSF on Renneke's behalf. "It is by working closely with our users," says Sabelli, "and providing them with the backup they need—including joint proposals and letters of support—that NCSA can help achieve results beyond what the center's own resources and staff can do themselves."

The equipotential lines of two positive point charges at 9 volts surrounded by a border at 0 volts.



Even though the facilities available to Renneke are not yet ideal because his college lacks a remote network connection, he is eagerly taking advantage of Augustana's affiliation with NCSA. He is one of the growing number of educators who realize that supercomputers are no longer reserved for a select few, but will soon be a common tool in every area of inquiry.

Says Renneke, "The payoff is using a new set of tools—hardware, software, and video—to provide insight into a basic physical principle." ▲

Cooperative program underway

by Kathleen Robinson, Science Writer

Barbara Mihalas, coordinator of NCSA Scientific Institute Affiliates Program.

Basic software tools and packages do not exist in many strategically important areas of science—and in others, the commercially available software is inadequate or prohibitively expensive. As a result, research groups all over the country are developing their own software—often at considerable expense and often duplicating efforts done elsewhere.

To address this situation, Dr. Barbara Mihalas was appointed coordinator of a new NCSA Scientific Institute Affiliates (SIA) Program in February [see ***access***, March 1990]. Under the SIA program, research staff from national institutes and universities will work together to develop action plans for different scientific disciplines. They will define the types of computational support that could significantly improve their respective research environments and work to obtain joint funding for cooperative projects.

Seven institutes have joined the program already [see next page]. NCSA is developing relations with several other institutions.

Program goals

Scientific involvement from across the country and the research spectrum is vital, says Mihalas, "to assure that software being developed is of general use and also effective for the whole community. This is not an appropriate arena for competition. The need is for cooperation as we build a foundation of computational tools for research."

History has shown that it is possible to build for the needs of a large research community. For example, as computers first became widely available, researchers coordinated their efforts to develop mathematical subroutine libraries and computer languages that the entire community could use, regardless of specialization. A similar effort is needed now.

Larger and faster computers, coupled with major conceptual breakthroughs in many fields, have pushed investigative efforts in new and exciting directions. Research momentum is building, increasing the need for shared solutions to common problems. A rare window of opportunity exists to boost the progress of science with, as Mihalas puts it, "the technical expertise at NCSA and the knowledge and experience present in other universities and research institutes."

Mihalas' background

The appointment of Dr. Barbara Mihalas as coordinator gives the SIA Program a running start. Mihalas has a wide acquaintance with scientists in various institutes and research communities—as a result of personal research contacts and through her recent work on approaches to developing an effective prototype data management facility. NSF has granted her an award to initiate prototype work for large, permanently archived scientific datasets.

While studying data management issues, Mihalas visited a number of scientific institutes to investigate their local development efforts or their data handling requirements. In the process, Mihalas worked with researchers from a broad cross section of academic disciplines that included those with a tradition of computation and those just getting acquainted with computational resources and approaches.

Since 1985, Mihalas has been a research scientist at NCSA with an adjunct appointment in the UIUC Department of Astronomy. Her research in astronomy has included the study of internal gravity waves in astrophysical contexts, solar and stellar oscillations, radiation transport, and radiation-hydrodynamics.

Before coming to NCSA, Mihalas worked as an astronomer at Sacramento Peak (Solar) Observatory, run by Kitt Peak, and at NCAR. Through her research on internal gravity waves and in helioseismology as well as her work at NCAR, Mihalas has developed ties with many researchers.

Mihalas' eclectic background, familiarity with NCSA, and wide acquaintance with scientific institutes and research communities provide a broad foundation for the development and coordination of the SIA program. If your institute is interested in joining the SIA Program, contact Mihalas [see **NCSA contacts,** page 15]. ▲

First seven SIA members

Technical Education Research Center (TERC) is a nonprofit organization for improving the quality and accessiblity of education for students with diverse skills and backgrounds. Transferring current technologies to elementary and secondary schools is especially important to TERC, which strongly believes that children can learn in the right educational settings if equipped with the right tools. According to project director Dr. Cecilia Lenk, TERC plans to use NCSA's technology and expertise to develop educational approaches and software tools that will enable students to innovatively explore complex concepts like global climate change.

National Center for Computational Electronics (NCCE) is a "center without walls" for a national community of researchers from academia and industry who are working on large-scale simulations of electron devices. The center is headquartered at the Beckman Institute. According to Dr. Karl Hess, the director, interaction with NCSA has been a tremendous boon to NCCE because its visiting scientists can use NCSA's supercomputers. NCCE works actively with NCSA's Applications group to port key device modeling codes to the supercomputers and with the Software Tools and Visualization Services and Development groups on improving ways to view simulations of three-dimensional microphysical processes.

Space Telescope Science Institute (STScI) is funded by NASA and located at Johns Hopkins University in Baltimore, MD. It has numerous overlapping interests with NCSA's Astrophysics team and UIUC's Department of Astronomy. STScI's activities center around the Hubble Space Telescope, to be launched in April. Dr. Ronald Allen, head of the Science, Computing and Research Support Division, spends one day a week at NCSA to work with Mike Norman, Barbara Mihalas, and the BIMA project [see page 6] to integrate astrophysical data into computational and visualization tools at NCSA.

Center for the Analysis and Predictions of Storms (CAPS) is an NSF-funded Science and Technology Center that maintains close ties with Bob Wilhelmson, faculty adjunct scientist at NCSA, and his students. Dr. Kelvin Droegemeir, deputy director of research at CAPS, plans to work with NCSA and members of UIUC's Department of Atmospheric Physics to adapt NCSA workstation visualization tools for the needs of the atmospheric science community. Additional funding is now being sought for this customization. Future plans include holding a fall workshop at NCSA on Comparison of Numerical Methods for Nonlinear Flows with NCSA and the University of Wisconsin–Madison.

Institute for Theoretical Atomic and Molecular Physics at the Center for Astrophysics (CFA/ITAMP) is jointly sponsored by the Harvard-Smithsonian Center for Astrophysics and Harvard University and is another new NSF-funded Science and Technology Center. It was established in response to the need to rectify the "critical shortage of theorists in atomic and molecular physics at major universities thoughout the nation." The center's goals are to attract and train graduate students and to maintain an active visitors program for senior researchers as well as a strong postdoctoral program for potential new university faculty in astrophysics.

Research Institute of Scripps Clinic, Department of Molecular Biology, is located at La Jolla, CA. Researchers in the Department of Molecular Biology are investigating proteins to improve and develop pharmaceuticals. A member of the department, Dr. Phil Cohen, has a Monte Carlo protein dynamics code that is well suited for adaptation to the Connection Machine (CM-2). Under Cohen's direction, a postdoctoral candidate will probably spend time at NCSA for that purpose.

Institute for Theoretical Physics (ITP) is a major national center in theoretical physics for postdoctoral and long-term visiting members. It is located at the University of California at SantaBarbara; Dr. James Langley is the director. Chiefly the institute runs long-term research programs and workshops of several months' duration on selected topics in theoretical physics. For example, the institute is currently offering a semester-long helioseismology workshop.

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BIMA: Visualizing the universe at millimeter wavelengths

by William Dwyer, Graduate Assistant Writer

Radio telescopes enable radio astronomers to probe the unseen universe. The best radio images can be obtained by connecting several radio dishes into an array called an *interferometer*.

Construction of the largest, most flexible, and fastest millimeter-wavelength interferometer in the world will soon be completed by a coast-to-coast research consortium of universities—the University of California at Berkeley, the University of Illinois at Urbana–Champaign, and the University of Maryland at College Park.

Called the Berkeley-Illinois-Maryland Array (BIMA), the project has received pivotal support from NCSA through development of software that can turn the interferometer's large volume of raw data into useful images. Richard Crutcher, who is one of three BIMA codirectors as well as UIUC astronomy professor, heads up the software development effort as director of the Laboratory for Astronomical Imaging (LAI), which is funded by NCSA and the UIUC astronomy department.

To change the angular resolutions and to fully sample the Fourier series, radio-telescope dishes in the existing array are moved to different stations on rubber-tire transporters.

The "aperture-synthesis-array" (the technical name for the system) will record radio wavelengths in the millimeter range from the rotational transitions of molecules in space. BIMA astronomers will use this tool to study galactic structure, star formation, evolved stars, planetary atmospheres, solar activity, and comet composition.

Doing science in real time

Researchers using the BIMA system will be able to concentrate on scientific analysis rather than processing data. The planned mode of operation, Crutcher explains, will enable investigators to have a completely processed dataset ready for analysis within hours instead of the weeks or months required previously. Investigators will be able quickly to either determine that the experiment should be run again or begin analyzing their dataset.

The BIMA array, located in northern California, consists of radio-telescope dishes that can be moved to change the angular resolution (the smallest detail discernable). Each parabolic dish focuses radio signals on a receiver, which makes up the telescope. The original array's three 6-meter diameter dishes will be supplemented with three dishes that will be part of the new system scheduled to be completed in mid 1991. Crutcher says the new system will be about 10 times faster than the existing three-dish interferometer. By the end of 1991 the speed may be increased even more: NSF has indicated interest in providing funding to add three more dishes (making a total of nine) to the array.

Computer driven and controllable from either Berkeley, Maryland, or Illinois, the new interferometer will send data to NCSA for immediate processing and archiving. The processing arrangement for BIMA data is unique in that it will be a complete system for collecting, distributing, processing, and storing data.

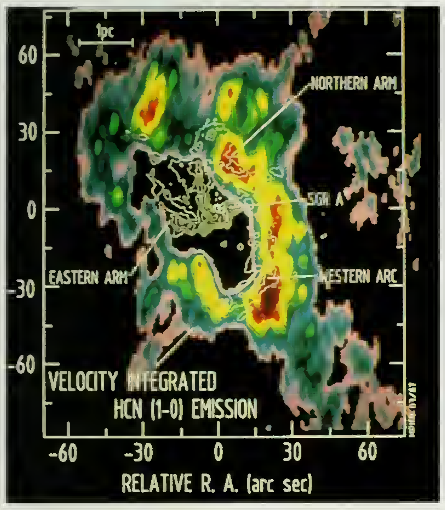
BIMA technology

BIMA, with its six or more dishes and sensitive 2,000-channel receivers, will produce enormous quantities of data. Timely processing requires supercomputers, according to NCSA Research Scientist Mike Norman. He says there are two main thrusts to the project—the science and the technology. "The technology is really what NCSA is involved in at the moment."

Radio telescopes, as the name implies, are designed to receive the longer wavelengths of the electromagnetic spectrum. To see the details in an object, radio telescopes must be correspondingly larger than their shorter-wave collecting cousins, the more familiar optical telescopes. When data from many dishes are combined appropriately—thus making it an interferometer—the array functions like one large telescope, whose diameter and angular resolution correspond to the separation of the dishes.

The BIMA array can be tuned to millimeter wavelengths between 1 and 4 millimeters. The instrument spreads the wavelengths so the various spectral lines, which provide information about the object being observed, can be analyzed. A spectrometer separates the signal into eight "windows" to observe eight spectral lines simultaneously.

Unlike optical telescopes that focus light waves on the eye or on photographic film (or more often now on digital processing equipment for display on a monitor), the receivers on



Produced with MIRIAD software, this image of center of Milky Way galaxy shows radio continuum emission from hot gas (contour map) surrounded by cold, dense gas (color raster image).

radio interferometers treat the incoming radiation data mathematically. Norman says these data must be Fourier inverted and retransformed thousands of times to make a clean image—hence the CRAY-2 supercomputer requirement.

Software developed for BIMA

Crutcher explains that inherent instabilities in the equipment and natural instabilities in the atmosphere make fuzzy images. The consortium wanted software developed to clean up the images.

Robert Sault, NCSA postdoctoral research associate, developed the WERONG software specifically for radio continuum mapping. This software has already been used to create several "supermaps" of such strong radio sources as Centaurus A and the center of our own galaxy [see photo above]. Supermaps, Norman explains, is hyperbole for maps as large as 4000 x 4000 pixels. Norman and Sault animated the creation of a supermap of hot gases in the center of the Milky Way Galaxy at SIGGRAPH'89 as part of NCSA's televisualization-by-satellite demonstration [see ***access***, September–October 1989].

According to Norman, the primary focus is now on MIRIAD (Multichannel Image Reconstruction, Image Analysis, and Display). "We're on the threshold of releasing a production version of MIRIAD for all the scientists working with BIMA," he says. Also developed at NCSA by Sault with contributions from BIMA partners at Berkeley and Maryland, this software package is used to calibrate data and correct instability errors. Norman refers to a MIRIAD-produced image that was used for the August 17, 1989, cover of *Nature*. The image was produced from data collected by Sundararajan Sukumar (NCSA postdoctoral research associate) and Ronald Allen (then chair of UIUC astronomy department, now at the Space Telescope Science Institute and visiting professor at the Beckman Institute) at the Very Large Array radio telescope in Socorro, NM.

The consortium also requested the development of higher quality software designed for the X Window System to better visualize data obtained from the BIMA system. Eng-Whatt Toh, student programmer in the NCSA Software Tools Group, has been modifying NCSA X DataSlice [see ***access***, July–August 1989] for visualizing the radio-source data. Toh has added the ability to access BIMA datacubes, which have two spatial dimensions and a third dimension that represents the radial velocity of the source molecules. Using data from the Orion nebula, Toh demonstrated this new technique in February for the Berkeley-Illinois-Maryland MIRIAD development group.

Networking

BIMA data can now be transferred between consortium members and the array by NSFNET, but Crutcher says that NCSA's share of this high-speed network is insufficient for real-time interaction with the array. However, Crutcher and Norman are working with an NCSA program that may use the BIMA project as one of several applications on a national gigabit-per-second network testbed.

Involving collaboration among AT&T Bell Laboratories and several universities, this program will include funding from DARPA and NSF through the Corporation for National Research Initiatives (NRI).

The testbed network—called XUNET (Experimental Universities Network)—will link universities at Berkeley and Urbana-Champaign as well as the University of Wisconsin–Madison and Bell Laboratories in New Jersey.

BIMA researchers at UIUC

In addition to Crutcher and Norman, BIMA researchers at UIUC include astronomy professors Lewis E. Snyder and Kwok-Yong Lo; postdoctoral researchers David Adler, Bart Wakker, and Robert Sault; research programmer Harold Ravlin; and NCSA Director Larry Smarr.

Snyder, the discoverer of many important interstellar molecules, is using the array for astrochemistry studies, comet studies, and the study of the structure of molecular clouds. Crutcher is studying dense molecular clouds and the processes by which they form new stars. Lo—who leads an effort in making the superconductor-insulator-superconductor (SIS) junctions for use as detectors for the array—is studying the general structure of galaxies and the nature of the center of our galaxy. Norman, as head of NCSA's Astronomy and Astrophysics team, is involved in software development for LAI [see also ***access***, May–June 1989]. Smarr was instrumental in getting LAI startup funds for equipment and supplies.

NCSA's efforts have demonstrated its willingness to work with the astronomical community, according to Norman. And he expects NCSA to continue developing new resources for astronomical research. Observations by BIMA astronomers, Crutcher predicts, will provide a better understanding of the formation and evolution of stars, the nature of galaxies, and the origin of the universe. ▲

Solving the Einstein equations with numerical methods

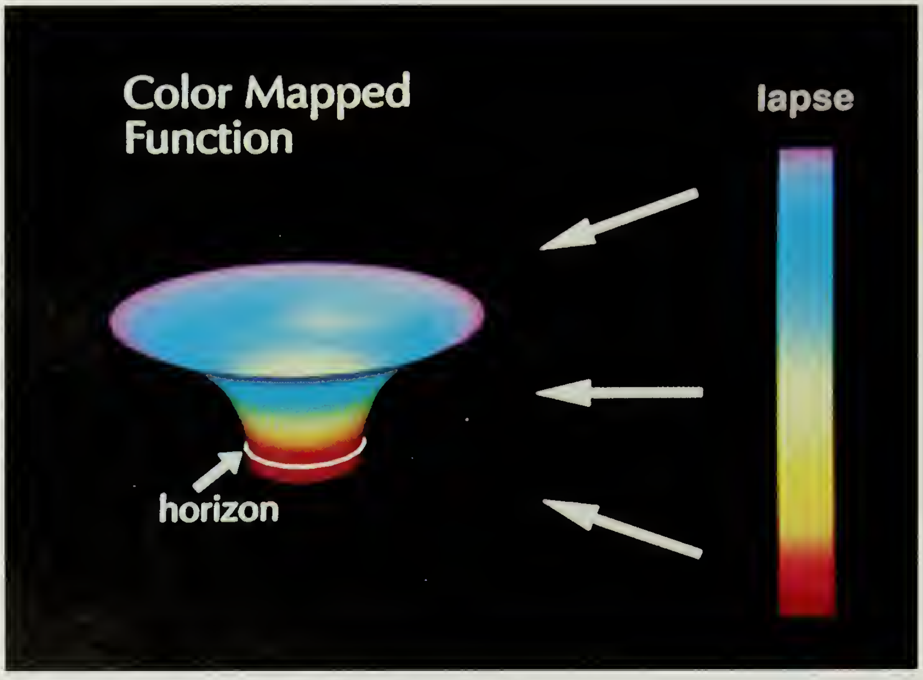
by Kathleen Robinson, Science Writer

Although most researchers use NCSA facilities from remote sites, some of the world's scientific pioneers are to be found within the NCSA Interdisciplinary Research Program housed at the Beckman Institute.

Dr. Larry Smarr, NCSA director and a leader in the field of numerical relativity, heads a research group at NCSA in numerical vacuum geometrodynamics—a discipline devoted to the study of gravity in the absence of matter. Others in the NCSA numerical relativity group are research scientist Dr. David Hobill, research associates Dr. Roger Ove and Dr. Ed Seidel, and graduate students David Bernstein and John Towns. They work with Dr. Steve Christensen's quantum gravity group at NCSA and collaborate with Dr. Andrew Abrahams of Cornell.

These researchers use numerical methods for obtaining solutions to the Einstein field equations—coupled nonlinear partial differential equations that describe gravitational fields in curved spacetime. These extremely complex equations have eluded full solution for 75 years.

About 20 years ago it became apparent that many of the important problems in relativity could not be addressed exclusively by analytic means. As a result, numerical approaches began to be employed. Numerical relativists now apply advanced computer technology and modern computational algorithms to the problems of relativistic gravitation.



The curved space surrounding a black hole can be visualized using an embedding diagram. Here, one spatial dimension is suppressed so that a ring represents a spherical surface. In this image the lapse function that determines how rapidly clocks keep time is colored red for the slow and blue for the fast clocks.

Three problems

Smarr and his numerical relativity group at NCSA are focusing on three theoretical problems.

The first is to study the effect on a black hole of a passing gravitational wave. A robust two-dimensional code has been constructed that shows small-amplitude oscillations remaining after the gravitational wave has encountered the black hole and moved on. The pattern produced by the numerical code agrees to within a few percent with analytic results calculated from perturbation theory. But, the code cannot accurately calculate the nonradiative part of the gravitational field for a long simulation without expending nearly 100 hours of Cray CPU time. The group plans to investigate using an adaptive mesh algorithm to increase accuracy.

A second, more difficult problem involves the formation of a black hole by the implosion of a strong gravitational wave. Preliminary calculations seem to indicate that if the amplitude of a gravitational wave is large enough, then self-gravitation can cause it to collapse and form a black hole. The group plans to modify the code that currently calculates the evolution of pure gravitational radiation so it will run longer with large-amplitude waves. The goal of this study is to learn how the nonlinearities of general relativity can turn a transverse radiative field into the longitudinal field of a stationary black hole.

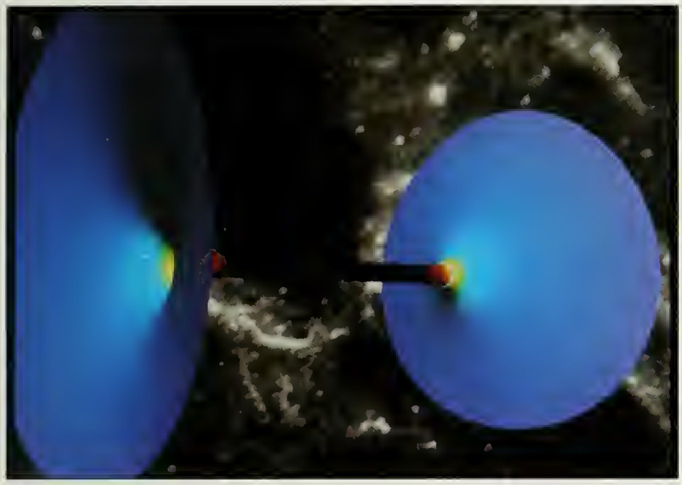
A third problem involves the head-on collision of two black holes. In 1976 Smarr wrote the first successful two-dimensional code for two colliding black holes. This code ran on a CDC 6600. Now, using the CRAY-2 supercomputer at NCSA, the group will run a more sophisticated code to look at the same problem. In addition, a new code will be developed to simulate the collision of *spinning* black holes, which is expected to produce a very different waveform signature. Says Smarr, "This problem will be substantially more complex than any other we have studied so far."

Symbolic manipulation

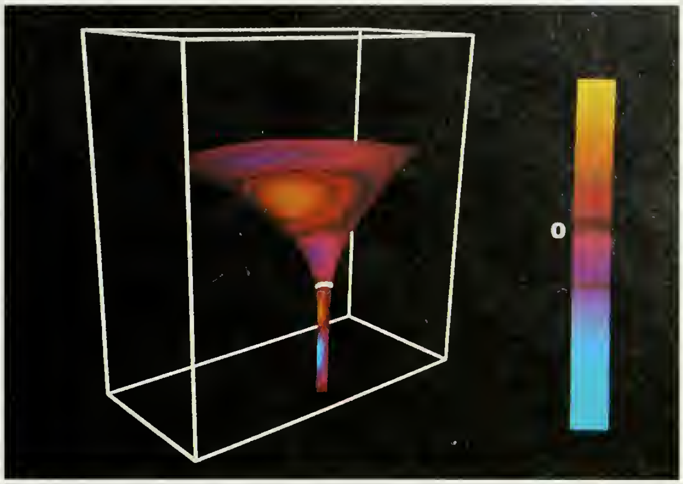
The relativity group at NCSA is investigating the use of various finite differencing schemes, gauge conditions, adaptive grids, and alternative variables to solve the field equations.

The relativists at NCSA have written and adapted numerical relativity codes for the CRAY X-MP and CRAY-2

This embedding diagram shows how the proper distances are stretched along an extended cylinder by choosing a time coordinate that avoids the singularity at the black hole's center.



A cutaway of an embedding diagram shows an oscillating black hole with high-frequency color map of the emitted gravitational wave amplitude.



systems, the Alliant FX/8, the CM-2, and a Myrias SPS-2. The group is now developing codes capable of running on the next generation of large-scale parallel machines.

They have successfully used the symbolic manipulation packages Macsyma, *Mathematica*, and Maple to derive the field equations and generate Fortran code for the complicated expressions that appear in their relativity codes. Says Smarr, "Use of symbolic manipulation has saved us enormous amounts of time. It is clear that as the codes of numerical relativity become more and more difficult to handle, the relationship between symbolic and numerical computations will become increasingly important."

As the interface between numerical and symbolic manipulations becomes stronger, the group expects that packages such as Math Tensor, now being developed by Steve Christensen (NCSA research scientist) and Leonard Parker (of the University of Wisconsin), will be useful not only for the coding process but also for post-production analysis.

Young field

Numerical relativity is a relatively young discipline; however, it is growing rapidly. This growth was seen during the NCSA-sponsored conference, "Frontiers in Numerical Relativity,"

Solving *continued on page 16*

General relativity—75 years

Nearly a century ago the German mathematical physicist Hermann Minkowski suggested that space and time should be understood as comprising a single four-dimensional continuum, called spacetime. Albert Einstein proposed that the presence of matter causes spacetime to be distorted, or curved, and that we experience this curvature as gravity.

Einstein developed the general theory of relativity to explain—through the use of complex, non-Euclidean geometry—how a given distribution of matter affects the curvature of spacetime. (The term *relativity* refers to the concept that there is no absolute motion in the universe, only relative motion.) Einstein's theory involved 10 coupled nonlinear partial differential equations—the "field" equations—that have yet to be completely solved 75 years later.

One reason for the field equations' complexity is that, according to the theory, the source of a gravitational field (the mass of an object) varies with the object's speed relative to the frame of reference in which it is found, so the value will be different at different points in spacetime.

Another reason for the complexity is that the equations are nonlinear: the results of changes in one variable can unexpectedly affect the values of other variables. Since the equations are coupled, the situation quickly becomes intractable using standard mathematical methods.

During the first 40 years in the history of general relativity, researchers were able to construct analytic solutions to the Einstein equations by making certain assumptions that simplified the complexity of the field equations. Unfortunately only a limited number of these solutions had any physical relevance. In the mid 1960s, the most powerful digital computers were located in government and industrial research laboratories, so the first attempts at constructing numerical solutions to the Einstein equations began at those installations. Those efforts were hindered both by a lack of sufficient computer power and an incomplete understanding of the geometrical nature of gravity. The latter problem was overcome in the late sixties when methods of modern differential geometry were used as tools for studying the mathematical structure of the Einstein equations. For the construction of realistic three-dimensional solutions, the former constraint remains an obstacle even today.

During the early 1970s, a few undaunted researchers were able to use the available computational power to solve a simpler version of the Einstein equations—namely, that involved the linearized perturbations about a fixed analytic solution. About the same time, armed with new insights provided by analytic methods and the line

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General relativity *continued from page 9*

of CDC-6600 and 7600 computers available only at government laboratories, Larry Smarr and his coworkers (notably Kenneth Eppley and James Wilson) successfully constructed the first singularity-avoiding, fully nonlinear numerical solutions using very crude grid spacings and very basic numerical techniques.

In the decade that followed, numerical relativity was practiced mainly by those with access to computers at government laboratories or foreign locations. The few existing researchers began refining their two-dimensional codes with more sophisticated numerical methods. This process, along with the inevitable increase in computational power, has led to more accurate and stable codes capable of studying such phenomena as black hole dynamics, neutron star formation, supernova explosions, and the evolution of the early universe. It was not until the 1980s—with the establishment of the national supercomputer centers—that the world's most powerful computing machines were made available to larger numbers of academic users.

Today previous problems associated with supercomputer access have been virtually eliminated and numerous young researchers have entered the field. While code refinements continue, efforts are being directed toward the development of three-dimensional codes that will predict the gravitational wave forms emitted from realistic astrophysical processes. These codes will eventually require the computing power available in future generations of supercomputers in order to obtain an accurate catalogue of gravitational wave sources and their wave profiles. Urgency is associated with such an undertaking since NSF will be supporting a multimillion-dollar project aimed at the construction of gravitational wave detectors based upon a design that uses very large, precise laser interferometers.

Through the collaboration of experimental and numerical relativists, a new branch of astronomy called gravitational wave astronomy is expected to be established by the year 2000. This will open a new window onto our universe.—*David Hobill, NCSA research scientist, contributed to this article and sidebar.*

Industrial Program

Partners discuss high-performance computing

by Rich Ingram, Caterpillar On-site Representative

Riaz Abdulla of Eli Lilly and Company addresses the first session of the industrial partners' roundtable meetings.

The rewards of being an industrial partner at NCSA amount to much more than having access to supercomputing cycles, software, and experts. By establishing a presence at NCSA, industrial partners are able to explore new tools and the effect high-performance computing can have on industrial research and product development.

To foster communication among the seven industrial partners, center staff, and other researchers, the industrial partners at NCSA have initiated a series of roundtable meetings open to all researchers. Each partner will make a presentation at one of the first seven meetings to introduce themselves. The corporate on-site representative will summarize his or her corporation's activities relating to NCSA or to computing in general.

Once the introductory series listed below is completed, biweekly roundtable discussions will continue on timely topics of interest.

February 22	Riaz Abdulla of Eli Lilly and Company
March 8	John Luranc of FMC Corporation
April 5	Larry Ray of Eastman Kodak Company
April 19	Margaret Nadworny of Motorola Inc.
May 3	Rich Ingram of Caterpillar Inc.
May 17	Jim Rieke of Dow Chemical Company
May 31	D'Arcy Randall of Amoco Corporation

All roundtable meetings are scheduled to be in Beckman Institute. Industrial representatives, academic researchers, and NCSA staff will be future speakers. ▲

Franklin Institute honors Smarr

by Jarrett S. Cohen, Public Information Specialist

NCSA Director Larry Smarr will receive the Delmer S. Fahrney Medal of The Franklin Institute on May 1, 1990, in Philadelphia, PA. The official letter of notification states that "this award is made for your leadership in helping to establish a national supercomputing program in the United States, and for your contributions to the development of programs for their use."

Fahrney, the medal's namesake, was a rear admiral in the U.S. Navy who endowed an award for "providing a climate in which scientific processes can be furthered," according to Charles F. Penniman, Jr., secretary of The Franklin Institute's Committee on Science and The Arts, which selects the medalists. Fahrney served as Committee secretary for 16 years and endowed the medal in 1975.

Past recipients of the Fahrney Medal include Peter Raven of the Missouri Botanical Garden, Mary L. Good of Allied-Signal Corporation, and William A. Nierenberg of the Scripps Oceanographic Institute.

Established during the Industrial Revolution, the Committee was a pioneer organization in the U.S. for evaluating inventions, said Penniman, who described it as an "engineering consulting service." The Committee on Investigations was founded in 1825 and was later renamed Committee on Science and The Arts.

Today, with "engineering invented and a patent office in place," the Committee's primary purpose is awarding medals for excellent work. These awards uphold The Franklin Institute's role in scientific education and, Penniman said, "the advocacy of curiosity."

The Committee on Science and The Arts is made up of 60 men and women from academic and industrial laboratories across the Delaware Valley. Among its members is cosmologist and NCSA supercomputer user Dr. Joan Centrella of Drexel University, Pittsburgh, PA [see **NCSA *News***, March 1987].

In addition to the Fahrney medal, Smarr will receive a certificate and a paper that evaluates the importance of his work. During the awards ceremony, held in the Benjamin Franklin National Memorial at the Institute, this will be one of several medals awarded. The keynote speaker will be Presidential Science Advisor D. Allan Bromley. ▲

Upcoming NCSA workshops and conferences

Finite Element Workshop
May 19–20
For more information, contact Ilhan Dilber, industrial consultant, at (217) 244-1973 or idilber@ncsa.uiuc.edu (Internet) or 13024@ncsavms (BITNET).

Molecular Dynamics Calculations Workshop
June 11–15
For more information, contact Nora Sabelli, senior research scientist, at (217) 244-0644 or nsabelli@ncsa.uiuc.edu (Internet) or 10241@ncsavms (BITNET).

Networking and Supercomputing Conference
late September
For more information, contact Charlie Catlett, manager of Networking, at (217) 333-1163 or network@ncsa.uiuc.edu (Internet) or network@ncsavms (BITNET).

Affirmative action

by Virginia Hudak-David, Assistant Director for Administrative Affairs

NCSA was one of two recipients of an award for an outstanding affirmative action program. The award was presented at a UIUC meeting held February 28 that addressed affirmative action in nonacademic employment. NCSA Director Larry Smarr and Assistant Deputy Director Marcia Miller, formerly the manager of administration, accepted the award on behalf of the center. University of Illinois President Stanley Ikenberry addressed the group on creative affirmative action and human resource strategies to prepare for "Work Force 2000." NCSA is pleased to be recognized as a leader in nonacademic affirmative action on the Urbana campus and looks forward to continued success in this area. ▲

Newly designed training sessions

by Lyle Rigdon, Manager, Training

NCSA is committed to training the academic and industrial community in the use of high-performance tools such as the Cray supercomputers, the Connection Machine (CM-2) system, and NCSA software on desktop workstations. Training sessions also keep our academic and scientific institute affiliate representatives up-to-date and well versed in the activities of the center. On-site and remote workshops and seminars can be arranged.

Discussions with our industrial and academic users have led us to upgrade our training to reflect their comments and suggestions. We will continue to modify and enhance the program based on user feedback and comments. Please let us know how we can better serve *you*!

New user training

NCSA's new training organization is based on the cohesive set of modules listed below.

Applications Module. Topics include parallel sessions in at least three fields (finite element analysis, computational chemistry, computational fluid dynamics); overview of software in a field; steps involved to use software packages covered by the session; postprocessing capabilities of packages; comparisons of packages; and extensive hands-on laboratories.

Connection Machine Module. Topics include machine architecture; programming in C, Paris, and Fortran; frame buffer usage; data vault usage; and extensive hands-on laboratories.

Cray Introductory Module. Topics include introduction to UNICOS; intermediate UNICOS; NQS batch system; and extensive hands-on laboratories.

NCSA Introductory Module. Topics include overview of services, organization, staff, and facilities; basics of networking; history of NCSA; current and future plans; and reference to all materials and publications.

Visualization Module. Topics include overview of visualization; Cray graphics; HyperCard animation package; introduction to raster graphics; NCSA Scientific Visualization Software Suite; NCSA HDF; and media output.

These modules are organized into the following three training sessions:

- **Cray Applications.** This three-and-a-half-day session includes NCSA Introductory, Cray Introductory, Applications, and Visualization modules.

- **Cray Code Development.** This five-day session includes NCSA Introductory, Cray UNICOS Introductory, Cray Fortran/C Development, and Visualization modules.

- **CM-2.** This five-day session includes NCSA Introductory, Connection Machine, and Visualization modules.

Users are welcome to attend a portion of a training session if space is available.

Affiliates training

Training sessions for NCSA academic and scientific institute affiliates normally last five days and combine relevant portions of new user training modules. Major functions include:

- Introducing new affiliate representatives to NCSA and its facilities

- Updating representatives on new offerings and procedures

- Providing extensive training on various topics

- Encouraging affiliates to share ideas, stories (strategies), and suggestions

- Helping affiliate representatives get to know NCSA staff and whom to turn to for assistance

- Soliciting comments and suggestions from affiliate representatives

Outreach training

We will take NCSA training material on the road as needed and available. Outreach sessions may last from 2 hours to 3 days, depending upon users' needs and the availability of resources. A representative from NCSA and a coordinator from the remote site work together to customize each outreach session using some of the topics included in the new user training modules. Outreach training is available to both academic and industrial locations.

A comprehensive list of module agendas and suggested prerequisites is available from Training on request [see **NCSA contacts**, page 15]. Proposed training dates for 1990 are listed on page 16. ▲

New NCSA academic affiliate

Brown University
Providence, RI
Michael P. Russell
(401) 863-2617
mrussell@brownvm.brown.edu

Speakers announced for June computational chemistry workshop

by Nora Sabelli, Assistant Director for Educational Outreach

Plans are progressing for the Workshop on Molecular Dynamics Calculations on High-Performance Computers scheduled for June 11–15, 1990.

This hands-on workshop is aimed at research scientists who have basic knowledge of the field and need to become better acquainted with computational modeling strategies.

Speakers from academia and industry will discuss their experiences with several software packages, describe new methodologies, present comparisons between methods and parameterization schemes, and share troubleshooting hints and strategies.

The following speakers have accepted our invitation to participate in the workshop:

David Beveridge
Wesleyan University
J. Phillip Bowen
University of North Carolina–Chapel Hill
Gilda Loew
Molecular Research Institute
Ronald Elber
UIC
David Gorenstein
Purdue University
Eric Jakobsson
UIUC
Scott Kahn
UIUC
Joseph Klimkowski
Eli Lilly and Company
Clark Landis
University of Colorado
Nelson Rondan
Dow Chemical Company
Harrell Sellers
NCSA
James Shields
Eli Lilly and Company
James Snyder
Searle
Julian Terado
Purdue University

Topics include ab initio and semiempirical quantum chemistry calculations for force field parameterizations, force field fitting and comparisons, perturbation free-energy calculations, and solvation effects.

Calculations and laboratory exercises will be run on NCSA supercomputers using such software packages as GAUSSIAN88, AMBER, and CHARMm; on high-performance workstations with graphics front-ends loaded with CHARMm; and on Macintosh IIcx workstations with images downloaded from the Cray systems.

During open laboratories participants will work in teams on their own research problems. Lecturers, NCSA scientists, and software vendor representatives will be at hand to assist if necessary.

Between 40 and 60 participants are anticipated for approximately 20 self-selected teams. There will be a fee for the workshop; NCSA has asked NSF for financial support to waive the fee for academic participants. For more information, contact Nora Sabelli [see "Upcoming NCSA workshops and conferences," page 11]. ▲

Online notes

DOCVIEW simplifies online documentation searches

by Jim Ferguson, Industrial Consultant

DOCVIEW, an online documentation system for reading and indexing manuals, is now available on both the CRAY X-MP and CRAY-2 supercomputers at NCSA. DOCVIEW complements the short documentation found in man and help pages by providing entire documents for your reference.

DOCVIEW is designed to make large manuals accessible and usable online. The system is user friendly and easy to learn. Full-screen menus give you a quick overview of available commands, and each step in the system is supported by a multilevel help feature.

Large manuals are indexed online by inserting keywords into each document. Keywords delimit passages of each manual and describe the material in each passage. You look at a list of the keywords in a document and choose which keyword passage to view. Keyword lists are available in both alphabetical order and the order in which they appear in the manual.

Another helpful feature of DOCVIEW is that it can search for information across documents. Uncertain which manual to view, you can issue a find command that searches for a particular keyword through all documents in the system. You receive and then select from a list of possible documents, the associated keyword, and the passage length. The find feature uses a form of "fuzzy matching," so the keyword does not have to match exactly.

DOCVIEW was designed and written under a joint project by consultants at NCSA and at Cray Research Inc. (CRI). DOCVIEW is based loosely on the DOCUMENT program, which was designed at Lawrence Livermore National Laboratory and runs under the CTSS operating system. CRI is planning to release DOCVIEW with UNICOS 6.0, the next version of their operating system.

NCSA will be adding documents to the DOCVIEW system as they become available. Please see this month's ***data link*** for information on how to run DOCVIEW. ▲

New and updated online information

by Will Ridenour, Online Documentation Editor

The following help files, documents, and man pages have been added or updated as of March 5, 1990. This list updates the November–December 1989 NCSA *Online Documentation on the Cray Systems*. For a copy of this publication, contact Orders for User Publications and NCSA Software [see **NCSA contacts**, page 15].

UNICOS help files

topic name	**description**
calendar	*scheduled NCSA events*
consult	NCSA consulting office schedule
sac	Small Allocations Committee meetings
contacts	*whom to contact for specific information*
consult	NCSA consulting office location and phone
software	*the latest list of software on NCSA machines*

To access a help topic, enter **`help`** ***`topic`*** where topic is the name of the topic you wish to view.

UNICOS man pages

The man page descriptions below match word for word the online descriptions.

man page name	**description**
chemistry	
ampac	semiempirical molecular orbital analysis package
charmm21	macromolecular modeling package
chemistry	describes chemistry software
gamess	ab initio molecular orbital analysis package
mm2	molecular mechanics package
mopac	semiempirical molecular orbital analysis package
ranfold	predicts significance of RNA secondary structures
rnafold	folds RNA sequences
mathematics	
abaqus	finite element analysis program
lapack	describes linear algebra package
slatec	describes general-purpose math library

To access a UNICOS man page, enter **`man`** ***`manpage`*** where manpage is the name of the man page you wish to view.

ULTRIX help files

The following help topics have been installed on the VAX/ULTRIX system:

topic name	**description**
access	access to NCSA
calendar	scheduled NCSA events
catalog	NCSA *Technical Resources Catalog*
contacts	whom to contact for specific information
conversion	notes on the conversion from VMS to UNIX
finding-information	how to find information online
policies	NCSA policies for users
security	security tips for NCSA users
software	the latest list of software on NCSA machines
tapes	reading and writing tapes at NCSA
training	information on user training at NCSA

To access a help topic on either Cray system or the VAX/ULTRIX system, enter **`help`** ***`topic`*** where topic is the name of the topic you wish to view. ▲

New UNIX-based gateway

A VAX 3600 running ULTRIX was installed at NCSA in late March, and the VAX 11/785 cluster running the VMS operating system is expected to be removed in April. ULTRIX is Digital Equipment Corporation's BSD UNIX-based operating system.

This change was based on a survey of users, vendors, and systems analysts. The new, unified UNIX environment provides a consistent user interface across all tiers of the NCSA computing network.

The VAX 3600 ULTRIX system serves as a gateway for BITNET mail and file transfer and as a tape handling facility for the Cray systems. Other services, such as network communications, are provided by the terminal server and IP routers.

Licensing for the VAX 3600 permits a maximum of 16 simultaneous logons. All users can access the Cray systems directly via telnet or the terminal servers. You do not need to use the VAX gateway to access the Cray systems.

The NCSA VAX Migration Plan was sent to all users in March. For the most current information on the VAX ULTRIX system, refer to online help by entering **`help`**.

NCSA contacts

General information and machine access

NCSA receptionist
(217) 244-0072
FAX (217) 244-1987

Orders for user publications and NCSA software
Debbie Shirley
(217) 244-4130

NCSA ombudsman
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(217) 244-0633
13013@ncsavms (BITNET)
bottum@ncsa.uiuc.edu (Internet)

Anonymous FTP IP address
ftp.ncsa.uiuc.edu (128.174.20.50)

CM Sun front-end address
cmsun.ncsa.uiuc.edu (128.174.220.4)

CM VAX front-end
cmvax.ncsa.uiuc.edu (128.174.220.5)

Cray operations
(217) 244-0710

CRAY X-MP IP address
ux.ncsa.uiuc.edu (128.174.10.46)

CRAY-2 IP address
u2.ncsa.uiuc.edu (128.174.10.44)

Dialup access—2400 baud or less
(217) 244-0662

Dialup access—9600 baud
(217) 244-6733

NSF Network Service Center
nnsc@nnsc.nsf.net

NSFNET problems
(617) 873-3400

SRI-Network Information Center
(415) 859-3695
nic.ddn.mil

VAX/ULTRIX gateway addresses
ncsagate.ncsa.uiuc.edu
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ncsagate (BITNET)

Programs and mailing lists

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Visitors Program
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uadmin@ncsa.uiuc.edu (Internet)

Visualization Services and Development Group
Dan Brady
(217) 244-2003
14998@ncsavms (BITNET)
dbrady@ncsa.uiuc.edu (Internet)

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which brought together most of the world's numerical relativists. While 60 percent of the participants were graduate students or recent Ph.D.s, there was also a sizable representation of established researchers now looking to numerical computations for new insights into the Einstein field equations. Given the enthusiam and expertise of those entering the field, it would seem that the future of numerical relativity looks very bright. ▲

Training dates, 1990

May 21–25	New User Training—CM-2 *(tentative)*
June 4–7	New User Training—Cray applications
July 23–27	New User Training—Cray code development
August 20–23	New User Training—Cray applications
September 17–21	New User Training—Cray code development
October 8–12	New User Training—CM-2 *(tentative)*
October 22–26	Affiliates Training

Note: Dates are subject to change and class size is limited. You must register to attend.

To register: Academic users, contact Karen Gobble at kgobble@ncsa.uiuc.edu (Internet) or at (217) 244-4198. Industrial partner users, contact your representative at NCSA.

Additional information: Contact Lyle Rigdon, Training Program at (217) 244-3659 or 26818@ncsavms (BITNET) or lrigdon@ncsa.uiuc.edu (Internet).

Scientific visitors

Fouad Ahmad
Jan. 11–June 15, 1990
University of Wisconsin–Milwaukee
Engineering

Thomas Bouman
Aug. 1, 1989–Aug. 31, 1990
Southern Illinois University–Edwardsville
Quantum chemistry

Michel Caffarel
Nov. 3, 1989–Nov. 30, 1990
University of Paris
Physics

Ernesto Esteban
Sept. 1, 1989–Aug. 30, 1990
University of Puerto Rico
Physics

Phil Hardee
Mar. 12–16, 1990
University of Alabama–Tuscaloosa
Astrophysics

Almon Turner
Mar. 7–9, 1990
University of Detroit
Chemistry

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  by Will Ridenour
- Brookhaven Protein Data Bank online
  by Joe Golab
- X-PLOR available on the CRAY X-MP system
  by Joe Golab
- SLATEC source retrieval system available
  by Beth Richardson

To receive a copy of the current issue of ***data link***, contact the NCSA receptionist at (217) 244-0072.

Subscriptions

Mail to Tammie Hildreth, Information and Publications, NCSA ***access***,
152 Computing Applications Building, 605 E. Springfield Ave., Champaign, IL 61820.

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May–June 1990 vol. 4 no. 5

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Visualization

Still from "Landscape Dynamics of Yellowstone National Park." (Courtesy of NCSA Visualization Services and Development group, pages 1 and 3)

Fires over Yellowstone

by Kathleen Robinson, Science Writer

Whatever happened to Smoky the Bear? Once the stern symbol of aggressive national fire control policy, he has faded into the background as ecologists learn more about fire's vital role in the life of a forest. But too many people remember Smoky's message that all fire is bad.

Not necessarily so, insist the experts, with growing stacks of data to illustrate their new understanding. Fire plays a vital role in the dynamics of forest evolution. It quickly transforms fallen plant material—decomposing slowly in cool, dry forests—to essential nutrients that leach into the soil. Fire releases seeds from pine cones and opens the forest canopy so seedlings can get the sunlight they need. Fire fosters plant and wildlife diversity in forests that would otherwise become groves of similar trees—all the same few species and all the same age, homes for a relatively narrow range of wildlife.

Most forest fires are small (a few hectares) and are over in hours. (One hectare equals approximately 2.47 acres.) But historical evidence shows that cataclysmic fires, like those experienced in the United States during the summer of 1988, recur every 200 to 400 years and are necessary to the continued vitality of a forest. The problem is one of communication: How to convince the public—and public policy-makers—that forest fires should not always be suppressed.

One way to do this may be visually, by illustrating the facts and figures that form the growing body of ecological data about the history and role of fire in the forests. A visualization project recently completed at NCSA does just that—bringing 300 years of Yellowstone fire history to life. A segment from the study aired on the PBS show "Yellowstone on Fire" on "Nature" in April. When some actual fire footage and narration are added,

Fires *continued on page 3*

Attention

See page 14 for changes to training dates and topics. This updates earlier listings and the April NCSA events calendar.

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Dear Readers:

With this issue, ***access*** will come to you bimonthly.

Publication dates for the remainder of 1990 are as follows: July–August, September– October, and November–December. You will receive each issue of the newsletter in the second month of publication.

As in the past, ***data link*** will follow the same production schedule as ***access.***

Melissa LaBorg Johnson
Managing Editor

NOTE: Italicized titles indicate sidebars or boxed information. Boxes may not follow the topics of the heads under which they fall.

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Connection Machine is a registered trademark of Thinking Machines Corporation.
CM-2 is a trademark of Thinking Machines Corporation.

Abbreviations

CRI	Cray Research Inc.
DARPA	Defense Advanced Research Project Agency
IRP	Interdisciplinary Research Program of NCSA
NCAR	National Center for Atmospheric Research
NCSA	National Center for Supercomputing Applications
NSF	National Science Foundation
UIC	University of Illinois at Chicago
UIUC	University of Illinois at Urbana-Champaign

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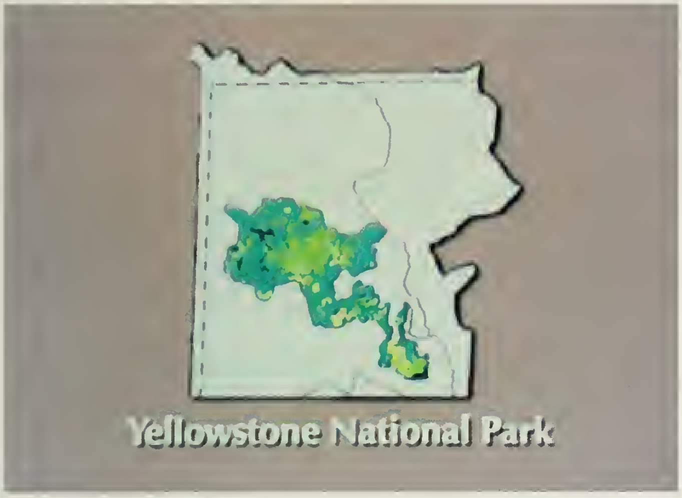
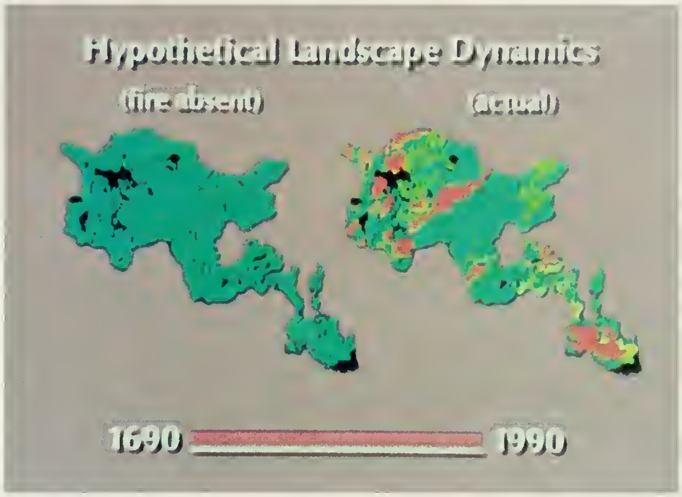
605 East Springfield Avenue, Champaign,
Illinois 61820

Map of Yellowstone National Park. Colored area indicates portion studied and keyed with color-coded patches of vegetation (see page 14).



Comparison of park's vegetative growth (1690–1988) after fires occurred (right) as opposed to simulated result (left) of no fire outbreaks during the same period. Red indicates area of 1988 fires.



***Fires** continued from page 1*

the videotape may be used as an orientation tool in the visitors' center at Yellowstone National Park.

Dr. David Kovacic is an ecologist in the Department of Landscape Architecture at UIUC. He studies the effects of disturbance—whether natural or manmade—on different ecosystems. Several years ago he was impressed with elk migration studies that used video animations to communicate the data. "I tried the same technique in a talk I gave and was overwhelmed by the impact that visual data presentation made on experts in the field. I figured if *these* people get excited, it would be a good way to communicate with the general public. I knew Bill Romme [associate professor of ecology at Fort Lewis College in Colorado] and Don Despain [ecologist at Yellowstone National Park] had a lot of data compiled on fire history in the Yellowstone area. It seemed to me that it might be useful to visualize that," recalls Kovacic.

Dating long-dead fires

Just how can anyone know what the past 300 years of fire activity were in an area where no written records exist? Romme and Despain first constructed a map of forest patches containing trees of similar age using low-level aerial photographs that cover nearly 130,000 acres in Yellowstone National Park. Then they visited every patch larger than 5 hectares and collected nondestructive core samples from five to ten dominant lodgepole pines, the most common tree in the Yellowstone area. They also cut cross sections from any fire-killed trees in each patch.

Together, the core samples and slices allowed the researchers to determine the age of the trees in each patch of forest and when fires had passed through the patch. Minor, survivable fires were recorded by scars on certain rings in the living trees. Even in the absence of fire-scarred trees to date, they could infer the occurrence of major fires just from the existence of even-age stands. Lodgepole pines usually germinate after the heat of a fire has liberated seeds from the cones they bear. (They also produce open cones that seed freely in the absence of heat, but relatively few of those seedlings survive because of insufficient sunlight.) After a significant fire has opened the forest canopy and liberated seeds from the cones, conditions are ripe for mass germination, and a new stand of lodgepole pines is started.

Romme and Despain reconstructed the percentage of trees of different ages for each period of their study. They also charted the occurrence of fires over the years, the severity inferred from the amount of scarring found in tree cores and from dead trees. This information they plotted out, with different numbers representing fires and the different age stands. Each printout showed the trees and fires at one point in time, but from the individual printouts it was difficult to gain a clear picture of the overall patterns of fire and growth. This is where Kovacic's use of color and animation came into the picture.

From Mac to Cray and back

Kovacic worked with NCSA visualization specialist Alan Craig to use code that Romme and Despain had employed. "When the original data came in from Kovacic, I created the preliminary images using NCSA Image on the Mac," says Craig. Kovacic obtained a small grant of Cray time through the Academic Affiliates Program, so Craig and Kovacic converted the original code to run on the CRAY X-MP/48 supercomputer to see what additional insights could be gained from the data.

"The data matrices were so big that Romme and Despain could only run their analysis at large intervals—say, 20 or 25 years. We took the data up to the Cray where we could look at it on a yearly basis," says Kovacic. "Not only did we visualize the past 300 years of fire history at Yellowstone, we also asked the Cray to show what would have happened to the diversity if there had been *no* fires."

***Fires** continued on page 14*

Monte Carlo methods on the CRAY X-MP

by Randall Graham, Science Writer

Visiting Research Scientist Michel Caffarel gambles mathematically to learn more about the electronic structure of molecules and thus their chemical and physical behavior. The CRAY X-MP/48 supercomputer is his "gaming table" and electrons his "dice."

Specifically Caffarel works with the Schrödinger equation, the basic mathematical equation for describing quantum properties of molecules. He employs Monte Carlo techniques to solve the equation—and that's where the gambling metaphor comes in.

"Monte Carlo methods," says Caffarel, "consist of using an analogy between the probability densities inherent in quantum mechanics and the probabilities of gambling to generate electron distributions in molecules. This is really just a mathematical trick, but it is a very efficient one for computing real physical properties of molecules."

Caffarel treats electrons as point particles and moves them randomly on the CRAY X-MP system. The Cray takes millions of snapshots of the electrons while they are moving and then averages the information revealed. This enables Caffarel to determine real physical properties of a molecule being studied.

Unfortunately Monte Carlo currently requires too much computer time to be practical for large molecules because finding a precise average requires too many snapshots.

The problem lies partly in the nature of electrons. Electrons generate complicated structures that become more difficult to simulate as the number of electrons increase. Caffarel's mission is to improve present Monte Carlo methods to make them more efficient. If shortcuts can be developed, working bigger systems will become practical with Monte Carlo techniques.

By injecting information already known about a molecule into the erratic motion of the electrons, the same average can be found with fewer snapshots and less computer time. Streamlining computational methods to shorten computer runs is one of Caffarel's primary objectives.

Customizing molecules

Solving the Schrödinger equation to a high degree of accuracy for any molecule is like hitting the jackpot in gambling. A wealth of information suddenly pours forth, such as the molecule's geometry and reactivity. Armed with this information, scientists can predict how a molecule or individual element will bond with others and even what properties the new molecule will have. The hope is that eventually scientists will be able to custom-design molecules with high-performance computers—incorporating desirable properties while then excluding undesirable ones.

Research scientists Michel Caffarel (left) and David Ceperley (right).

"The ability to determine how molecules will interact is very important," says Caffarel. "We could someday build molecules that have never been imagined before—developing new, specialized materials. All basic technologies are based on molecules or atoms." For example, Caffarel envisions a much more rational way of designing highly selective pharmaceuticals that heal the body without harming healthy cells.

It is also possible that a better understanding of the electronic structure of high-temperature superconductors via Monte Carlo methods may assist in their development. In the field of electronics, these methods could be used to design a molecule that is an electronic device, such as a transistor. Such a breakthrough might shrink electrical components by a huge factor.

Computing large systems

"We hope to determine or even choose the properties of a new molecule before ever going to the lab to actually produce it," Caffarel explains. "Developing a new substance on the computer rather than mixing things together in a lab by trial and error could save developers a fortune. Therefore, it is important to find more efficient methods of making this computation because of the important possibilities for predicting new structures and new materials."

Such exciting possibilities have not been realized, and Caffarel can't say when—or if—they ever will. Presently high-quality Monte Carlo simulations of the Schrödinger equation have been done for molecules with as many as ten electrons—water, for example—and that is an accomplishment. But this does not come near to the simulations needed to decipher the properties of truly complex electron systems, and every field of modern science seems to work primarily with large molecules.

Other mathematical techniques have been used to solve the Schrödinger equation for molecules with more than ten electrons (ab initio methods), but those methods have stalled before reaching molecules large enough to have widespread scientific interest. Monte Carlo techniques represent a new initiative for solving the equation—one that Caffarel and his peers hope will surpass other techniques.

Following his goals

Caffarel has been pursuing his goal for nearly six years. He began using Monte Carlo techniques as a graduate student at the University of Paris, France, where he earned a Ph.D. in physics in 1987 at the age of 25. Prior to that, he obtained an undergraduate degree in physics at the University Paul Sabatier in his hometown, Toulouse. For the past three years he has worked on quantum Monte Carlo at France's National Center for Scientific Research (CNRS), which employs roughly 30,000 people at various sites.

In November of 1989, Caffarel began a one-year stay at NCSA and the UIUC Department of Physics as a visiting research scientist under a NATO grant. He came to NCSA primarily to work beside Research Scientist David Ceperley and benefit from Ceperley's extensive experience. "David is one of the leading authorities on quantum Monte Carlo simulation," says Caffarel. "He has worked with many methods already, so he saves me time by keeping me from pursuing things that don't work. In three months here I've accomplished as much as I would have in a year at home."

NCSA's facilities and staff have proven to be a pleasant surprise for Caffarel as well. "Computational facilities here are excellent," notes Caffarel. "It's unusual to find two Crays and a Connection Machine on the same site. It is also easy to get help if you run into problems because the support people are quite available."

No packaged software exists for Caffarel's computations, so he writes his own code and uses codes written by Ceperley. He works off the CRAY X-MP system from a Mac IIx computer in his office at the Beckman Institute. The supercomputer is his laboratory. Caffarel hopes to use the Connection Machine and investigate the potential advantages of massive parallelism for his code.

"I'm really a strange hybrid of physicist and mathematician," Caffarel states. "I have to know some math to work my problems, but I also need to know physics to set the constraints of the problem. This is not a pure applied math problem."

Though progress can sometimes be slow, Caffarel is not easily discouraged. Like Edison who is said to have discovered 10,000 ways a light bulb would not work before finding the one way that it does, Caffarel pursues his goal—often working long hours. "At this point, it's impossible to know for sure if there is a way for Monte Carlo to make the Schrödinger equation workable for large systems. But if it isn't workable, I want to know that too. Even *that knowledge* would be very valuable. I intend to pursue it either to greater efficiency, or until I know for certain that it can progress no further." ▲

Erich Bloch visits NCSA

Erich Bloch (left standing), Jim Bottum (center), and Larry Smarr (right) observe while Crystal Shaw (left foreground) and Ray Idaszak (right rear) demonstrate the capabilities of the Numerical Laboratory in the Renaissance Education Laboratory.

Erich Bloch, outgoing director of NSF, spent a day at NCSA and toured the facilities in mid-March. Together with NCSA Director Larry Smarr who hosted the visit, Bloch observed research in progress and talked to a number of staff members.

"When NCSA was launched in 1985 with a five-year grant from NSF, its primary function was to make supercomputer cycles available to academic researchers," said Bloch. "This has been augmented by a research effort using the supercomputer as a base, spanning many disciplines from astrophysics to biology and engineering. The work on visualization, in particular, is impressive.

"Another unforeseen but valuable addition to the mission of NCSA is its industry program, transferring the application of supercomputer know-how to industrial companies to enhance their competitive position in the marketplace."

Concluded Bloch, "Service, forefront research, and technology transfer are mutually supportive activities in this vibrant university center." ▲

Communicating the global ideas of science

by Jarrett Cohen, Public Information Specialist

"NCSA has led me back to the very questions that led me away from research in the first place," says David Curtis, new associate director for Information and Publications.

Curtis grew up in London where he was born. "In England, the education system forces you to specialize even before you get to college," he says. Already at 16 he was placed on a science track. So before leaving school, Curtis took advanced-level examinations in biology, chemistry, and physics.

He went on to study biochemistry and chemical pharmacology at Queen's College, University of Oxford. Curtis describes his years there as similar to graduate school in the U.S.—studies were exclusively devoted to his chosen subject. His Ph.D. work in biochemistry at the University of Sussex differed from that in this country because there were no courses—and the research and dissertation counted for everything.

Despite having been published in some prestigious journals, Curtis became less and less engrossed with the details of science and more so with its global ideas—the "big picture," as he calls it. "I became interested in learning less about more, rather than more about less," Curtis says.

The result was that shortly after getting his Ph.D., Curtis decided against continuing his research career.

"That was not an easy decision, having invested the better part of my twenties in it," he says. "However, I remained fascinated by the essential questions posed by science and sought to communicate them to a wider audience."

Communicating science with television

Curtis began to recall his long-held interest in photography and the visual arts in general. Over time these interests led him to seek work in television.

David Curtis meets with the Information and Publications group.

Curtis made some efforts at breaking into television in England, but he says his career did not take off until heading west to New York City on the urging of his wife Ina, a native of that city. After working one and one-half years as a free-lance writer specializing in medical videos, in 1983 Curtis found the outlet for which he had been searching—a new series produced by New York City's PBS station WNET-TV called "Innovation."

" 'Innovation' broadcast the latest developments in science, technology, and medicine," Curtis says. "It was designed for an educated, lay public."

Curtis began with "Innovation" as an associate producer. Two shows and two years later, he was promoted to a full producer. Among the many topics he covered are the Human Genome Project, marine pharmacology, noise pollution, the mathematical imagination, AIDS and the blood supply, and the search for extraterrestrial intelligence. Through a show in the series on scientific visualization, "In the Image of Nature," Curtis first encountered NCSA.

"In the Image of Nature"

Soon after researching the program in January 1989, Curtis came to NCSA because of its reputation as a pioneer in the burgeoning field of visualization. Curtis says that he was fascinated by the concept of the Renaissance Team—"the convergence of art and science and the meeting of different disciplines to probe nature in all its complexity."

Donna Cox, UIUC associate professor of Art and Design and creator of the Renaissance Team, was Curtis's first contact at NCSA. "I flew out here, and Donna Cox picked me up at the airport," he says. "She was incredibly helpful. We worked out two days' shooting in one afternoon. The actual shooting went very smoothly."

For the program, Curtis interviewed Cox and profiled her work in Renaissance Teams with Eastman Kodak Co., the first NCSA industrial partner; and with UIUC astronomer/NCSA Research Scientist Mike Norman and radio astronomer Jack Burns of the the University of New Mexico.

The program also featured UIUC meteorologist/NCSA Research Scientist Bob Wilhemson's storm modeling visualization. NCSA Director Larry Smarr's enthusiasm for computational science and visualization—new ways of doing and communicating science—particularly excited Curtis about NCSA.

Curtis's next project was a two-part production on the Human Genome Project. "The programs focused heavily on the need for automation and developing intelligent software to make sense of the data," he says. Producing this show helped him realize that centers such as NCSA would be critical to the success of the project. This further increased his interest in NCSA, but as he says, "I had to put it on a back burner."

A "coincidence of interest"

After seven years on the air, funding for "Innovation" ran out in the summer of 1989, and Curtis returned to independent work as a consultant for science-oriented video production. In a twist of fate, his first client brought him right back to NCSA.

AT&T produced an in-house video magazine *Directions* that was distributed to staff worldwide. Curtis was hired to produce a segment on the AT&T Pixel Machine, among whose users were Kodak researchers based at NCSA.

"Around that time," Curtis says, "there was a coincidence of interest. Larry Smarr and Deputy Director Jim Bottum were looking for new directions for Information and Publications."

"Smarr said that I could do what I was doing [that is, video production] but in an ongoing and expanding framework. In a very real sense, NCSA offered an incredible opportunity to embrace science on my own terms, being able to communicate the excitement, the magic of doing science—not in little corners, but as collaboration," Curtis says.

New Directions for Information and Publications

As associate director for Information and Publications, Curtis hopes to take the group along new paths.

In addition to continuing its print publications, the group plans to hire a video producer to create a video magazine. Based on ***access*** and aimed at its readers, programs will report on the latest advances in computational science and visualization. Curtis says he does not want to "just report on what NCSA is doing or what individual researchers are doing, but also glimpse into the human side of doing science and explore its wider implications."

The division will also collaborate with NCSA's Educational Outreach activities, focusing on education at all levels from grade school up through the postsecondary level to the public at large. By employing video and eventually including interactive techniques, NCSA plans to reach these groups and thus aid the cause of science and computer literacy.

"There are no limits to our imagination, yet our ability to communicate remains biologically constrained. How we overcome this barrier is where technology comes in," says Curtis. "Thanks to supercomputing and visualization, we can tap our imagination and share our visions as never before. The results are indeed profound—new ways of communicating and doing science that can cross geographic and cultural barriers."

Carrying out NCSA's mission for the 1990s, the Information and Publications group aims to explore interactive technologies of communication, which "will be with us into the next century," Curtis says. In time, these will be coupled with expanding electronic pathways—eventually gigabit networks—which will make information available digitally on a national, even international, scale.

"I want to see our division anticipate and adapt to this emerging technology," Curtis says. "It is not going to be easy and happen overnight. Rome was not built in a day, but a start has to be made." ▲

NQS changes in response to CRAY-2 users

On March 19, NCSA installed key changes in the Network Queueing System (NQS) for the CRAY-2 supercomputer. The changes are based on valuable input from our users as well as our own thorough analysis of how the CRAY-2 supercomputer was handling the increasing workload. During the first 2 months of this year, NCSA analyzed the CRAY-2 system turn-around problem, surveyed users about the problem, and took steps to begin solving the problem by implementing the new NQS configuration.

NCSA is very enthusiastic about the new NQS system. Initial results indicate that the new NQS is living up to its promise.

As part of the new system, we are developing an array of software tools to help users and NCSA monitor its performance. The resulting information will also enable users to estimate how long it will take to complete a job. Users have found the new system much more responsive with more predictable job turnaround than in the past.

As part of NCSA's ongoing monitoring of the Cray systems, statistics will be available online on the Crays in the directory /usr/local/doc/stats.

We at NCSA feel that we have learned enormously from our efforts to understand and improve the CRAY-2 NQS system. We are grateful to our users for helping us provide the best service possible.

To find out more about the new NQS system, enter:

```
help nqs
```

For further details, see "Changes to NQS on the CRAY-2 system" in the May–June issue of ***data link***.

Plans are underway to analyze and install a similar NQS configuration on the CRAY X-MP/48 system soon. ▲

Peer Review Board allocates supercomputing time

by Patricia Wenzel, Manager, Client Administration

NCSA encourages researchers to submit proposals for either Cray system (CRAY X-MP/48 or CRAY-2) or the Connection Machine (CM-2). Time is available immediately on the CRAY X-MP/48 or the CM-2, but there is a short delay until October for CRAY-2 time.

The CRAY X-MP can support additional allocations immediately. Plans are underway to analyze and install on the CRAY X-MP an NQS configuration that is similar to the NQS on the CRAY-2.

The CRAY-2 supercomputer continues to be allocated and used to capacity. The new NQS system has improved the system's turn-around time (see page 7).

Allocations approved at the March Peer Review Board meeting follow:

Donald Backer, U. of California at Berkeley, *Millisecond Pulsar Search in the Galactic Anticenter,* CRAY-2, 200 Service Units (SUs).

Scott Barnett, Northwestern U., *Monte Carlo Simulations of Heteroepitaxial Crystal Growth,* CRAY X-MP/48, 150 SUs.

Joan M. Centrella, Drexel U., *Numerical Relativity and Cosmology,* CRAY X-MP/48 and CRAY-2, 400 SUs.

Geoffrey Chester, Cornell U., *Quantum Simulation of Condensed Matter,* CRAY X-MP/48, 500 SUs.

Marvin Cohen, U. of California at Berkeley, *Quantum Theory of Clusters and Solids,* CRAY X-MP/48, 880 SUs.

Monica Olvera de la Cruz, Northwestern U., *Linear and Circular Polymer Gel Electrophoresis Studies,* CRAY X-MP/48, 100 SUs.

Ahmed Ghoniem, MIT, *Vortex Simulation of Turbulent Flow,* CRAY X-MP/48, 800 SUs.

Mark Gordon, North Dakota State U., *Potential Energy Surfaces and Dynamics for Reactions of Bicyclobutanes,* CRAY-2, 320 SUs.

Lorella Margaret Jones, UIUC, *Methods for Separating Quark and Gluon Jets,* CRAY X-MP/48, 50 SUs.

Malvin Kalos, Cornell U., *Path Integral Monte Carlo (PIMC) Simulations of Quantum Solids and Fluids,* CRAY X-MP/48, 300 SUs.

Arieh Konigl, U. of Chicago, *Studies of Dynamical and Radiative Properties of Astrophysical Jets,* CRAY X-MP/48, 180 SUs.

Richard Martin, UIUC, *Electronic Structure of Condensed Matter,* CRAY X-MP/48, 950 SUs.

Bernard Matkowsky, Northwestern U., *Numerical Study of Stochastic Dynamics,* CRAY X-MP/48, 50 SUs.

Dimitri Mihalas, UIUC, *Studies of Stellar Envelope Opacities,* CRAY X-MP/48 and CRAY-2, 825 SUs.

Ken-Ichi Nishikawa, U. of Iowa, *Particle Simulations in Magnetospheric Plasmas,* CRAY-2, 100 SUs.

Vijay Pandharipande, UIUC, *Nuclear Theory,* CM-2, 100 SUs.

Samuel Paolucci, U. of Notre Dame, *Direct Simulation of Turbulent Natural Convection in a Cavity,* CRAY-2, 100 SUs.

George Schatz, Northwestern U., *Theoretical Studies of State-to-State Chemistry,* CRAY X-MP/48 and CRAY-2, 250 SUs.

Michael Schlesinger, UIUC, *Research on Greenhouse-Gas–Induced Climate Change*, CRAY X-MP/48, 495 SUs.

Huseyin Sehitoglu, UIUC, *Finite Element Analysis of Fatigue Crack Closure,* CRAY X-MP/48, 100 SUs.

C. M. Soukoulis, Iowa State U., *Molecular Dynamics Studies of Film Growth,* CRAY X-MP/48, 100 SUs.

Ronald Taam, Northwestern U., *Hydrodynamical Processes in Binary Star Systems,* CRAY X-MP/48, 136 SUs.

Brian Thomas, UIUC, *Three-Dimensional Fluid Flow and Flow Analysis of Continuous Casting of Steel Slabs,* CRAY-2, 50 SUs.

Nien-Hwa Wang, Purdue U., *Molecular Interactions in Biochemical-Sorbent Systems,* CRAY X-MP/48, 300 SUs.

Jerome Weiner, Brown U., *Computer Simulation of Atomistic Models for Rubber Elasticity,* CRAY-2, 200 SUs.

Henry T. Y. Yang, Purdue U., *Finite Element Simulation of Metal Forming and Cutting Processes,* CRAY X-MP/48, 10 SUs.

March PRB Meeting

Number of proposals	29
CRAY X-MP only	17
CRAY-2 only	8
CM-2 only	1
Combination of above	3

	X-MP	CRAY-2	CM-2
Hours requested*	7979	7895	800
Percent SUs allocated^	76%	19%	12%

* These figures reflect what is allocated for the coming year only. They do not include SUs for years two and three of multiyear requests.

^ Some allocations were deferred pending requests for additional information from researchers. These will be acted on prior to the next meeting if possible. Deferred allocations are not included in these figures.

Vendor-partner workshop on CFD tools

by William Dwyer, Graduate Assistant Writer

Engine combustion, electronic cooling, pipe corrosion, furnace design, aerodynamics, plume analysis, rocket motor analysis, crystal growth, and effluent dispersion are just some applications for computational fluid dynamics (CFD) analysis tools—the topic of a March workshop for CFD software vendors and NCSA industrial partners. The audience of about 50 attendees at Beckman Auditorium had a more narrowly focused range of applications in mind. "The people here want to know chemical-processing–type codes," said Tim Whitley of Cray Research Inc. (CRI).

Jeff Simon, assistant director for the NCSA Industrial Program, told workshop participants that there were three goals behind the workshop: to explore the CFD tools available on NCSA's Cray systems, to discuss industrial partner interest in CFD tools, and to discover the direction CFD tools are headed.

According to Michael Engelman, president of Fluid Dynamics International, "CFD codes are not black boxes that blindly and unerringly reproduce physics." He concluded that CFD codes are "a viable and powerful tool for analysis of fluid flow." Engelman was one of three vendors' representatives who gave presentations on CFD software codes.

Representatives for the other vendors—Creare.x Inc. and CHAM of North America—discussed their products with representatives from five NCSA industrial partners: Eli Lilly and Company, Motorola Inc., FMC Corporation, Dow Chemical Company, and Caterpillar Inc.

Positive response from all

Creare.x Inc. representative Zahed Sheikh said the workshop was an excellent idea. "It's the first time we've had a chance to see our competition face-to-face," he added. Engelman, who heartily endorsed the format for the workshop that was developed at NCSA, said the highlight was getting feedback from the industrial partners. Steven Rawnsley of CHAM said that he welcomed the chance to demonstrate his software. The three vendors concurred it was a good opportunity to meet with the partners.

Whitley of CRI said the workshop offered a great way to get answers to the partners' questions all at once instead of incrementally. Jack Waldvogel of Motorola Inc. said the workshop proved "very fruitful. Technical issues got just as much time as sales issues because of the scientific environment at NCSA."

The vendor presentations were followed by a presentation by Michael Folk, senior programmer for NCSA's Software Tools Group. In response to questions from the floor, Folk discussed plans to develop tools for doing vector representations. His talk was followed by a vendor panel discussion moderated by Kent Misegades of CRI. On the following morning, the three vendors and CRI demonstrated their software in the Renaissance Educational Laboratory (REL) at the Beckman Institute.

The idea for the workshop came from Dow Chemical Company's onsite representative, Jim Rieke, who commented that it "was a very successful experiment." Margaret Nadworny, Motorola's engineering applications liaison, praised Rieke for the idea and "its effective and timely implementation. It was one of the more useful and informative workshops I have attended," she said. "Having no experience with any of these codes prior to the workshop, I am more confident with the information I am providing to my users. It is my hope that such a format is as beneficial to the vendors in coming to understand NCSA and the Industrial Program here."

The workshop allowed Rieke and the Dow engineers to compare two finite difference codes and one finite element code. "It was instructive to compare various aspects of the pre- and postprocessors as well as the visual representation of results," Rieke said. "It also became increasingly clear that no single CFD code will adequately cover the wide range of problems that we are interested in; the conference provided a good starting point for additional comparisons and evaluations."

Caterpillar Coordinator, Rich Ingram, said the workshop was "well worth the time for the nine Caterpillar engineers that attended...the participation of Cray Research and the opportunity to view their new visualization tool, MPGS, was also very valuable to those who attended." Ingram said the interaction at the workshop led to several follow-up meetings with the vendors, including a visit to Fluid Dynamics International.

NCSA developing software

NCSA's Folk said there were many questions and comments following his talk—for example, users wanting NCSA DataScope or NCSA DataSlice to be made to work with 3D data. He said there is also much interest in tools and a file format for 3D mesh data. NCSA is currently developing two codes: a V-set format for the Hierarchical Data Format (HDF) software and Polyview, the IRIS-based program for viewing such data.

Folk said users also want to be able to translate different file formats to HDF to make visualization possible, and they want more features in NCSA Image for tieing colors to numbers. "CFD seems to be a promising area for developing visualization tools," he said.

Nadworny complimented Jeff Simon and Ramesh Jayaraman, NCSA CFD team leader, on their effective orchestration of the sessions. She looks forward to other workshops and suggests that future workshop topics include structural analysis, electromagnetic analysis, process simulation at the factory level, and simulation languages. ▲

Bad news/good news in U.S. education

by Kathleen Robinson, Science Writer

> "Now here, you see, it takes all the running you can do, to keep in the same place. If you want to get somewhere else, you must run at least twice as fast as that."
> —White Queen to Alice in *Through the Looking Glass*

The *bad* news is that plodding U.S. educational practices are badly out of step with the breathless pace of change in science and technology today. The *good* news is that concerned individuals at every level—from the president of the neighborhood PTA to the president of the United States—are now convinced that changes in the system are absolutely vital. With such a consensus, technological nation's schools—from kindergarten through the post-graduate college level—*may* prove able to keep abreast of technological change into the next century.

NCSA recently installed 16 Macintosh workstations in local grade schools.

At the moment, though, too few young people are training for careers in science and technology to meet projected needs for the future, many experts warn. Moreover, many students perceive they lack access to new technologies. And in many cases, they actually do. Worse yet, more and more students fail to develop the analytic and deductive tools needed to make informed decisions in an increasingly technological world.

NCSA's educational outreach

NCSA is working hard to help all that. Under the leadership of Dr. Nora Sabelli, NCSA senior research scientist and assistant director of Educational Outreach, a multipronged program for sparking interest among many levels of students is being implemented even as it is being designed. "Education exists at NCSA as an integral part of most, if not all, of our activities," Sabelli says.

Pilot projects now underway in local schools will be developed into curricula for national dissemination. Other existing projects involve educators from campuses across the country, while many projects are being proposed for development.

Projects underway

As the following list shows, NCSA's efforts in the area of educational outreach are affecting education at all levels. Projects already underway have:

- Installed 16 Macintosh workstations (including 2 Mac IIs and 2 LaserWriters) at 3 local elementary schools and trained teachers in their use. Classroom experience and teachers' comments will be used to design plans for other areas.
- Helped elementary and middle school science teachers in the local community write proposals to use workstations and networks in active science projects designed by their students.
- Started collaboration with local high schools to develop a new chemistry curriculum with visualizations and simulations that the students manipulate.
- Worked with the local community college to develop the first graphics and visualization certification program in the U.S. [see **access**,

Local grade school children use the CM-2 in a science project.

May–June 1989]; 20 students are now completing their study.

- Opened the Renaissance Experimental Laboratory (REL) and made it available to local and visiting faculty. The REL contains 20 Silicon Graphics IRIS Super System personal workstations donated by Silicon Graphics. The lab is used on a regular basis to teach UIUC courses [see ***access***, May–June, 1989] and the community college visualization curriculum noted above.
- Participated in a lecture series for high school students and teachers on supercomputing. This is the second year of NCSA involvement—sponsored by an 8-county consortium of educational districts in Illinois. Approximately 70 students and teachers attended each of three Saturday sessions presented by NCSA staff members Nora Sabelli and Donna Cox and graduate student Harold Brooks.
- Offered workshops to introduce teachers to the use of workstation tools and supercomputers for visualizations and simulations. One educator who attended last summer's 2-week workshop, David Renneke of Augustana College, uses the CRAY X-MP/48 in a physics course [see ***access***, April 1990].
- Established plans for teams of students and faculty to visit NCSA and work in NCSA's facilities. These teams will then support and encourage others on their own campuses.
- Began to develop strategies and workshops to provide graduate students and researchers with computational science concepts/methods.
- Began to seek funding for educators to spend their sabbaticals developing course modules that incorporate high-performance computing into undergraduate curricula.

Projects under development

Portable class modules on computational science and engineering concepts that educators can use to quickly update their courses are in the development stage. Testing and documentation of these course modules will be done by undergraduate and minority colleges affiliated with NCSA.

Plans are in the thinking stage for the creation of a national program of industrial research projects within the high schools; this program would be in collaboration with NCSA's industrial partners.

Also in the thinking stage is a library of visualized basic science concepts to build and enhance science curricula.

Projects in the proposal stage include collaborating with the Illinois Math and Science Academy to expand access to and education on high-performance computing to high school teachers statewide and collaborating with Jackson State University to develop a similar program for minority schools in Mississippi.

The goal of NCSA's outreach program is to promote, develop, experiment, and coordinate—not deliver, Sabelli says. NCSA has plans to develop resources that help universities, faculty members, and institutions provide a state-of-the-art environment for explorations, course development, and testing. ▲

SDSC workshop

Participants are invited to submit proposals for papers, poster sessions, panels, and demonstrations for the Volume Visualization Workshop that SDSC will host December 10–11, 1990 at San Diego, CA.

For more information, contact Charlotte Smart, SDSC, by telephone at (619) 534-5071 or by electronic mail at vvworkshop@sds.sdsc.edu.

NCSA software updates

by Jill Peacock, Editorial Assistant, and Jason Ng, Senior Programmer, Software Tools Group

NCSA's Software Tools Group recently released updated versions of various scientific software packages. These software programs are more versatile in their enhanced versions.

These packages can be downloaded via anonymous file transfer protocol (FTP) or purchased from NCSA. See the details below.

NCSA Layout 1.2 for the Macintosh permits batch capabilities that generate animation sequences on the Cray or other UNIX systems. You can create a batch mask in NCSA Layout, transport the animation template to the Cray, use the UNIX tool called Laybat to create an animation sequence on the Cray, and download that resulting sequence to the Macintosh for viewing in other software such as NCSA Image and NCSA ImageIP. Other new features include enumeration of each animated frame, multi-image display in animation frames, halftone printing, scrolling windows, canvas sizing, full overlay capabilities, and transparent text and colored background options. As in its previous release, NCSA Layout continues to help you make professional presentations and produce quality slides. Your layout may include several images annotated with grid lines and tick marks; text; color bars that display the range of the current palette; graphics from non-NCSA software such as MacDraw, PowerPoint, and PixelPaint; and a colored canvas. By loading or pasting user-defined color palettes into NCSA Layout, you can change the appearance of images and the colors in your text and canvas. Furthermore you can save a layout as a raster image that may be transferred to other machines or programs for photographing, animation, or display.

HDF Vset 1.0 is the latest storage scheme in HDF (Hierarchical Data Format). It can accommodate existing HDF data elements (for example, raster images, scientific datasets, palettes, and annotations) as well as varied, irregularly structured and nonuniform datasets of any size and dimension.

Specifically HDF Vset makes the following two features available to you: (1) All kinds of regular (array-type) and irregular datasets may now be stored in one HDF file. This includes mesh data, multivariate datasets, sparse matrices, finite-element data, spreadsheets, splines, non-Cartesian coordinate data, etc. (2) Related and diverse datasets can now be linked together hierarchically to form logical groupings.

The HDF Vset interface utilizes a simple data-description scheme; this description is then used as the format for data storage. To retrieve the data, all that is needed is a brief description of the data fields of interest. Partial access to data items and data fields may be specified, too. In addition, the linking feature forms "links" between storage elements. For the first time, logical groupings can be established within the HDF file.

Beta versions of Vset calling interfaces are available for C and Fortran on Crays/UNICOS, Suns, SGIs, and Vax/VMS.

NCSA CompositeTool 1.1 for the Sun Workstation is a simple, flexible program that allows the display and annotation of three types of 2D data—data (raster) images, contour intervals of a 2D data image, and vectors of 2D data—in a form suitable for generating presentation-quality 35mm slides from your Sun screen. NCSA CompositeTool allows you to overlay data with grid lines, XY axes, tick marks, and text titling; load a user-specified palette, display the palette color bar, perform screen dumps of selected portions of the canvas, and store and retrieve NCSA CompositeTool sessions for future use. HDF support that allows users to directly write commands and retrieve information via the HDF library [see ***access***, February 1990], is featured.

Obtaining NCSA's public domain software

If you are connected to Internet, you can obtain NCSA software by downloading it. You can also order all the above software except HDF Vset 1.0 through the NCSA *Technical Resources Catalog*, March 1990. If you are not connected to Internet, to obtain a copy of HDF Vset 1.0 call "Orders for user publications and NCSA software" [see **NCSA contacts**, page 15].

How to download: If you are connected to Internet (NSFNET, ARPANET, MILNET, etc.), you can download software, documentation, and source code (if it is available) at no charge from an anonymous FTP server at NCSA. See the *Technical Resources Catalog* for the procedures. If you have any questions about these procedures or the connection, consult your local system administrator or network expert.

How to order: To order software developed at NCSA, see the March 1990 *Technical Resources Catalog* for instructions. Order forms are included in the publication. If you want additional catalogs, contact the NCSA receptionist at (217) 244-0072. ▲

Visualizing solid-state semiconductors with PISCES IIb

by Scott Piette, Industrial Consultant, Industrial Program

Today the U.S. runs a tight, some say lost, race with Japan in the production of semiconductors and the ability to build better microchips for the computer industry. According to *The Economist* (quoted in the April 15, 1990 issue of *The Washington Spectator*), "Productivity growth in American manufacturing is well below that of any other rich country." Citing the failure of old industries under foreign competition, it is stated that new industries are following suit. "The electronic industry has been submerged by imports. Japan now produces more than half the world's semiconductors and nearly 80 percent of dynamic random access memory chips." In response to this challenge, U.S. semiconductor research and development is active.

Solid-state semiconductor analysis application programs simulate the behavior of new designs in solid-state devices, and they play an essential role in today's complex design of computer microchips.

Advantages of simulation

By converting the simulation output into images, research scientists are able to gain a better understanding of the behavior of their complex devices in ways that were previously impossible. Design problems can be identified and corrected *before* solid-state devices are committed to costly production runs by viewing the behavior of electrons as they travel inside solid-state devices and through buried structures.

Simulation techniques can also be used to explain the operation of the basic elements of today's semiconductor technology to new college students. By generating animation sequences of basic devices such as transistors, diodes, and SCRs (silicon controlled rectifiers), students can better understand the behavior of these devices as they interact with the animations.

Installed on the Crays

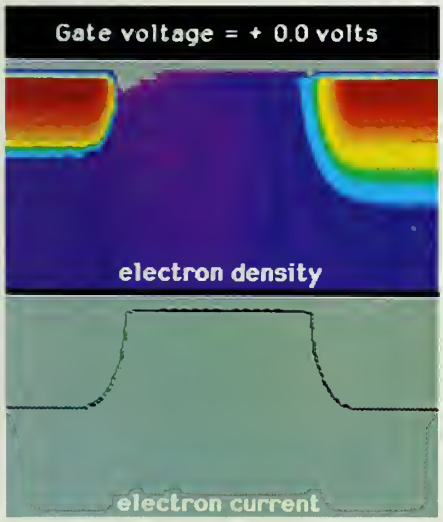
As part of the NCSA–Apple Computer Inc. Mac IIx Equipment Grant Program [see ***access***, July–August 1989], some NCSA staff members have been developing a visualization program called PISCES IIb for viewing the output from a solid-state simulation program. PISCES IIb is a two-dimensional simulation program from Stanford University. It is installed on both Cray supercomputers at NCSA and is available to the academic community at no charge.

Easy-to-use program

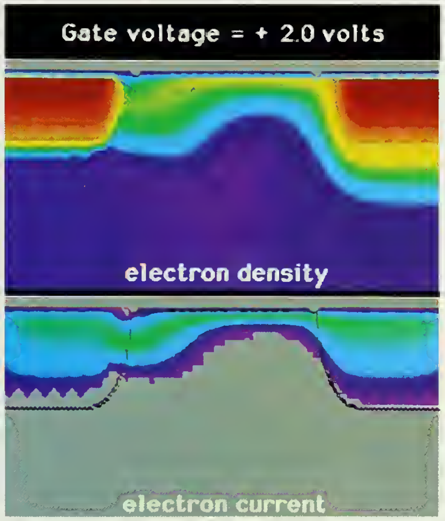
This visualization program is easy to use. For example, it converts ASCII output from PISCES IIb into NCSA HDF (Hierarchical Data Format) color raster images. These raster images are generated from each solution in the simulation output file. By generating a series of raster images, an animation can be made that shows the operation of a device being studied. Animations can be viewed by using the NCSA Scientific Visualization Software Suite for the Macintosh [see ***access***, July–August 1989] and NCSA X Image for X Window systems [see ***access***, July–August 1989].

The images on this page exemplify PISCES IIb's visualization output. Electron density and current inside a MOSFET transistor in operation are depicted. At the left below, the transistor starts in the off state (Gate = 0 volts). As the gate voltage is increased (center), the device starts to turn on (Gate = +2 volts) and heightens further (right) to a final voltage of +9 volts.

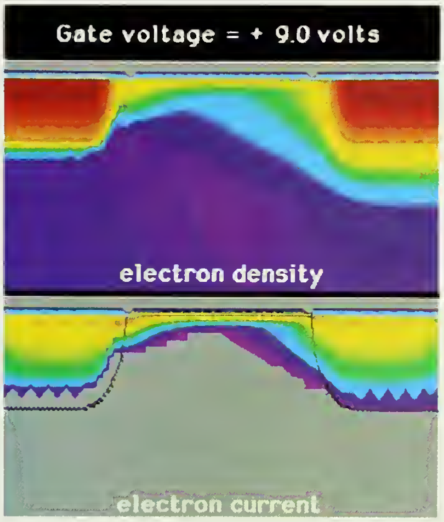
For more information on this utility, contact Scott Piette by electronic mail at spiette@ncsa.uiuc.edu (Internet) or 13042@ncsavms (BITNET) or by telephone at (217) 333-4221.



Transistor in off state (Gate at 0 volts).



Transistor starting to turn on (Gate at +2 volts).



Transistor in on state (Gate at +9 volts). (Photos courtesy of Scott Piette.)

Speedy CM-2

Through formulation of an algorithm and utilization of a special technique (virtual processing), the Connection Machine (CM-2) ran at the speed of 3.1 billion calculations per second. Virtual processing allows each processor to act as more than one.

Modifying a set of governing equations developed in 1938, University of Michigan graduate student Philip Emeagwali designed an algorithm to simulate petroleum reservoirs. Coupled with virtual processing, the code attained gigaflops-plus speed—small wonder. Emeagwali won the 1989 IEEE Gordon Bell Prize competition awarded this year.

This year's winning speed was three times that of last year's in what is regarded by some as the Olympic Games of supercomputing. According to Emeagwali, the supercomputer used by the winner is declared the "fastest supercomputer on earth."

Emeagwali used CM-2s located at NCSA, Lawrence Livermore National Laboratory, Argonne National Laboratory, and Thinking Machines Corp. ▲

Fires continued from page 3

Craig adds, "The code ran fast enough that we could ask questions as we went—what happens if we eliminate *this* fire, or *that* one?"

The results of the Cray output were written as NCSA HDF (Hierarchical Data Format) files, which were used with NCSA Image software on a Mac II to create the images that went into the final animation. Color represents stands of different ages in the images. As one watches the video, the effects of fire on the diversity of the forest are unmistakable.

A preliminary animation was done on a Mac II. But with the possibility of a national audience, Kovacic enlisted the help of Bob Patterson, postproduction supervisor of NCSA's Media Services. Using a Silicon Graphics Personal IRIS workstation, Abekas A60 and A64 digital disk recorders, Abekas A53-D digital effects machine, and a Calaway edit controller, Patterson created composite video images, layering the numerous visual elements to create a professional-quality videotape for communicating the complex facts about forest succession.

Each run of the animation contains 300 time segments—one for each year of study. Patches of vegetation studied by Romme and Despain are color coded on a map by age: yellow represents new growth to 40 years; light green, trees that are 40 to 150 years old; medium green, trees 150 to 300 years old; and dark green, trees over 300. Red patches, for fire outbreaks, flash on and off randomly over the area from 1690 to 1872. In the latter year, U.S. fire suppression policy began.

Before fire suppression, small, scattered annual fires led to diversity, shown by the map's mosaic of meadows, young forests, and old stands. In contrast, the same stands without fire show almost the entire region in dense maturity—a dark green blanket. During fire suppression times, there are smaller, fewer red patches than in the years fires occurred naturally. Yellowstone's forests grew less diverse as they became more flammable. The buildup of natural debris set the stage for the fires of 1988.

States Kovacic, "This project was really exciting. You can see static maps of the information, but this video animation puts it together in a form you'd never be able to see otherwise. When you see the forest dynamics through time you get a much different feel for what happens. It's a fantastic learning tool for scientists as well as the public." ▲

Revised 1990* training dates

July 23–25	Cray Applications Training**
August 20–24	Cray Code Development Training
September 17–19	Cray Applications Training**
October 8–12	CM-2 Training
November 5–9	Cray Code Development Training
December 3–5	Cray Applications Training**

You must register to attend NCSA Training. Class size is limited.

To register Academic users, contact Karen Gobble at (217) 244-4198. Industrial partner users, contact your representative at NCSA. Academic affiliates contact Kendra Reasor at (217) 244-1100.

For additional information Contact Lyle Rigdon at (217) 244-3659 or lrigdon@ncsa.uiuc.edu (Internet) or 815@ncsavms (BITNET).

*Note These dates and topics are subject to change.

**Applications will be in the fields of chemistry, finite element analysis, and computational fluid dynamics.

Gaussian newsletter

To establish better communication with Gaussian users, Gaussian Inc. will begin publishing a regular newsletter.

It will discuss updates, new implementations, future developments of the Gaussian system of programs, and user-group meetings and workshops.

Anyone who wishes to be on the mailing list should contact:

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CM VAX front-end
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ux.ncsa.uiuc.edu (128.174.10.46)

CRAY-2 IP address
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(217) 244-6733

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New and updated online information

by Will Ridenour, Online Documentation Editor

The following help files, documents, and man pages have been added or updated as of April 23, 1990.

UNICOS help files

Name	Description
access decnet	Information on DECnet access to NCSA
calendar high-performance	The NCSA High Performance Computing Calendar
finding-information	How to find information online
policies memory	Memory limits on NCSA machines
software	The latest list of software on NCSA machines
unicos memory	Estimating memory requirements for UNICOS jobs
unicos nqs	Information about the network queuing system

ULTRIX help files

Name	Description
access decnet	Information on DECnet access to NCSA
calendar high-performance	The NCSA High Performance Computing Calendar
conversion	Notes on the conversion from VMS to UNIX
finding-information	How to find information online
software	The latest list of software on NCSA machines

To access a help topic on either Cray system or ncsagate, enter: `help topic`
where *topic* is the name of the topic you wish to view.

UNICOS man pages

Name	Description
hsml	Describes sparse matrix library
recipes	Describes collection of math sub routines

To access a UNICOS man page enter: `man manpage`
where *manpage* is the name of the man page you wish to view.

UNICOS documents

See May-June ***data link*** for a list of recently installed Cray documents. ▲

data link contents

- Hot tips and topics
- Changes to NQS on the CRAY-2 system
- Running batch jobs under UNICOS
- Matrix multiplication benchmarks on the CRAY-2 system
- GAUSSIAN88 revisited
- X-PLOR now also on the CRAY-2 system
- Harwell Sparse Matrix Library available
- Numerical Recipes accessible from CFS
- Tools for network service study

To receive a copy of the current issue of ***data link***, contact the NCSA receptionist at (217) 244-0072.

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Mail to Tammie Hildreth, Information and Publications, NCSA ***access***,
152 Computing Applications Building, 605 E. Springfield Ave., Champaign, IL 61820.

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NCSA
National Center for Supercomputing Applications

access

the NCSA newsletter

July–August 1990 vol. 4 no. 6

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Supercomputers and the environment

Today there is a worldwide growth in environmental awareness.

This issue features three NCSA-affiliated scientific researchers who exemplify this interest in different approaches: Gregory McRae, whose charting of LA's pollution impacts policy-making; Almon Turner, whose modeling of ozone depletion aids researchers; and Phillip Austin, whose findings about clouds lend insight on global warming. Many other NCSA-affiliated researchers are working on aspects of global change—too many to mention in this issue. All are part of an international effort to husband the Earth now and for the future.

NCSA is providing supercomputing allocations and other services (such as software tools and video production) to environmental researchers as part of the federal mandate for attacking one of the Grand Challenges of the 1990s—prediction of weather, climate, and global change. NCSA plans to become an integration point for the emerging scientific emphasis on environmental studies.

Thanks to their unique abilities to analyze complex models of nature and visualize natural processes, supercomputers are playing a vital role in meeting the planet's environmental challenges.—*Fran Bond, Editor* ▲

Misty morning, White Mountains, NH.
(Photo by © David Riecks.)

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Abbreviations

ACM	Association of Computing Machinery
CRI	Cray Research, Inc.
NCSA	National Center for Supercomputing Applications
NSF	National Science Foundation
UIC	University of Illinois at Chicago
UIUC	University of Illinois at Urbana-Champaign

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Refining ozone (O_3) depletion models

by Randall Graham, Science Writer

Twenty years ago, ground-level ozone (O_3) was receiving a mostly bad press. At ground level, ozone is an air pollutant—a toxic, foul smelling, bluish gas that causes eye and respiratory irritation even at low concentrations. (The worst smog contains ozone at 0.3 parts per million.) Ground-level ozone is formed primarily by sunlight-induced reactions between auto and factory emissions and the common oxygen (O_2) we breathe.

But in the stratosphere, ozone is a lifesaver. It forms a blanket around the globe at a height of 10 to 30 miles and has the unique ability to absorb ultraviolet (UV) light from the sun. Without the ozone layer, much life on Earth would likely disappear because unblocked UV rays kill plant and animal cells from the bottom of the food chain up. Since even small amounts of UV light are thought to cause cell damage and induce skin cancer, recent advertising campaigns urge sun worshippers to wear sun blocking lotions.

Though ozone blocks the sun's UV rays, it is sunlight that starts its formation by breaking O_2 molecules into single atoms to join with other O_2 molecules. Unstable alone, they join with other O_2 molecules to form O_3. Similarly, sunlight breaks apart O_3, so ozone is constantly being created and destroyed in the stratosphere. Nature maintains the ozone layer through chemical equilibrium.

Manmade chemicals, the culprit

Manmade chemical pollutants have drifted slowly skyward and are now eating away at the vital ozone layer. The discovery of this problem in the late 1970s eventually resulted in a ban on aerosol propellants containing chloroflourocarbons (CFCs). Comprised of chlorine, flourine, and carbon, CFCs are extremely stable near the ground, but when they drift into the stratosphere where sunlight is intense, they break apart into highly reactive species that can destroy ozone. Although CFCs account for approximately 30% of ozone depletion and have received the most attention, other pollutants also consume ozone. Nitrous oxide (N_2O) diffuses upward from auto exhaust and breaks into destructive nitrogen oxide (NO) in the stratosphere. This accounts for 50% of ozone depletion. OH, or hydroxyl, also consumes ozone, but it occurs naturally from water and does not upset the ozone equilibrium. The addition of NO and chlorine (Cl) causes the imbalance.

In spite of the aerosol ban, CFCs have remained in use as refrigerants and synthetic foams, and they continue to be released into the atmosphere when the foams are burned or refrigerators and air conditioners leak. Used since the 1930s, CFCs take decades to drift into the stratosphere. Environmentalists worldwide want to ban CFCs.

The urgent need for a solution to the problem of pollutants and ozone depletion gained new momentum in 1985 when scientists discovered a large hole in the global ozone layer over Antarctica. Thinning of the blanket had been observed for years, but a hole was something shocking and new. It gaped as large as the United States during Antarctica's spring. Now the hole occurs every year. It closes in the summer and fall but returns each spring and appears to be growing.

An international 1987 treaty signed in Montreal calls for a 50% reduction in the production and use of CFCs by the year 2000. Some corporations, such as Nissan and AT&T (an NCSA strategic industrial partner), have made plans to comply with the treaty, called the Montreal Protocol, before the deadline. As part of a broad industrial effort to reformulate products to help protect the environment, Dow Chemical Co. (an NCSA industrial partner) phased out CFCs as blowing agents in Styrofoam insulation in mid-July 1990.

Ozone's three worst enemies

Almon G. Turner, professor of physical chemistry at the University of Detroit, has turned his attention to refining current ozone depletion models using the CRAY X-MP/48 supercomputer at NCSA. He believes an important step toward solving the dangerous ozone depletion problem is a better understanding of the chemical reactions involved.

Turner approaches the problem mathematically: "Our work is purely theoretical rather than experimental."

Turner calculates the physical properties of the reactant and product molecules in the three known ozone depletion cycles to determine the reactivity of each molecule. Since these depletion cycles occur simultaneously in an atmospheric melting pot, it is believed that they interact.

There are three primary cycles thought responsible for ozone depletion: the reactive chlorine (ClO_x) cycle, the reactive nitrogen (NO_x) cycle, and the reactive hydrogen or hydroxyl (HO_x) cycle. The species in these cycles may contain either one or two oxygen atoms, so x may be 1 or 2.

The reaction sequences for each cycle are essentially the same. Symbolically, the chemical equations look like this:

$$X + O_3 = XO + O_2$$
$$XO + O = X + O_2$$

The capital X in these equations should not be confused with the subscript notations in the cycle titles. Each cycle has its own species for X.

For the (ClO_x) cycle, X is Cl	$Cl + O_3 = ClO + O_2$ $ClO + O = Cl + O_2$
For the (NO_x) cycle , X is NO	$NO + O_3 = NO_2 + O_2$ $NO_2 + O = NO + O_2$
For the (HO_x) cycle, X is OH	$OH + O_3 = HO_2 + O_2$ $HO_2 + O = OH + O_2$

Refining ozone *continued on page 20*

Air pollution in the LA basin

by William Dwyer,
Graduate Assistant Writer

July and August begin the smog season for many southern Californians. But according to an air pollution researcher at Carnegie Mellon University, Pittsburgh, PA, the word *season* may give the wrong impression. In the Los Angeles metropolitan area, where national air pollution standards are violated about 200 days a year, smog is not seasonal. LA has one of the nation's severest pollution problems, and it spends $300 million annually on air quality control, says Gregory McRae, professor of chemical engineering and of engineering and public policy at Carnegie Mellon.

Although LA's inhabitants and visitors can attest to the visibility of smog, it's often what you can't see that can hurt you. Ozone, an invisible component of air pollution, forms from the interaction of sunlight and oxygen with chemicals emitted by automobiles, power plants, and factories that burn fossil fuels. Not only is breathing ozone harmful, it damages plants and many materials.

Visualizing data

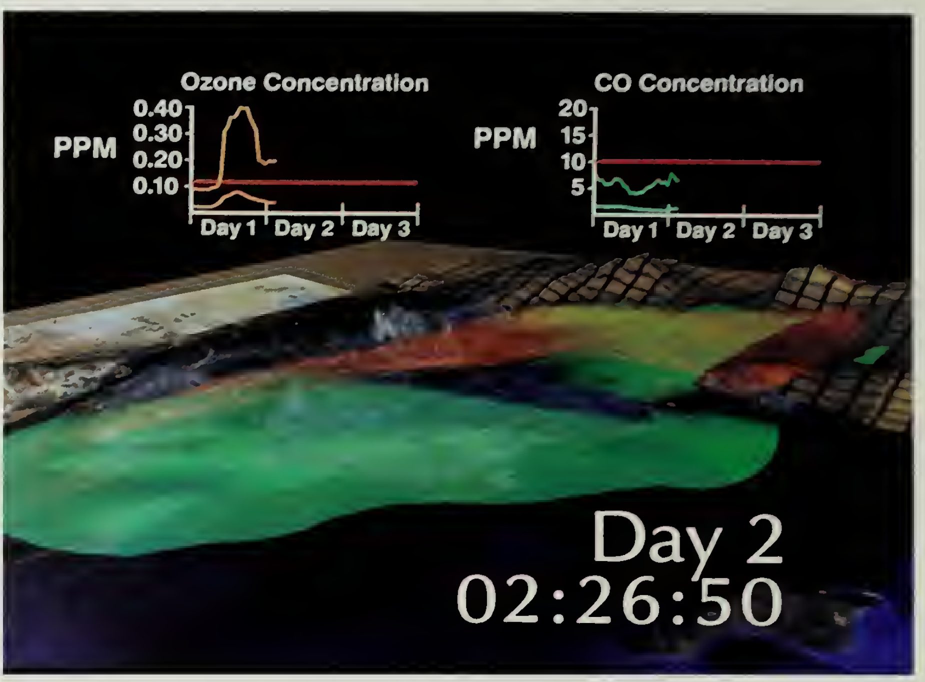
McRae is working with NCSA's Visualization Services and Development (VSD) group to make ozone and other pollutants visible to researchers and policymakers alike in a videotape entitled "Smog: Visualizing the Components."

NCSA Scientific Animators Michael McNeill and William Sherman incorporated McRae's pollution emissions data with Landsat photographic data and meteorological and elevation data from the Los Angeles area to produce two animated sequences on videotape. One sequence shows concentrations of ozone and carbon monoxide above a specific level in LA for a three-day period. The other shows movement and change in concentration of pollutants as determined by their production and dispersion by wind motion for the same three-day period. (See accompanying sidebar, page 5.)

According to McRae, NCSA's visualization attracts many people with varying interests—scientists, regulatory agency members, politicians, and industry representatives. McRae received the first version of the animated visualization while he was in Los Angeles in May. He said he "must have shown it 25 times" to various people at the California Air Resources Board; the South Coast Air Quality Management District, sponsors of the work; and at the Jet Propulsion Laboratory to researchers interested in visualization. "They're all uniformly impressed," he said. "[The visualization is] going to get an enormous amount of exposure." [Other funding sources for McRae's research include the Environmental Protection Agency (EPA); Cray Research, Inc. for computer time; and the Coordinated Research Council.]

Visualization impacts policy

"All you need to do is take one deep breath to understand the problem," explains McRae who moved from Australia to LA in 1975 to study environmental engineering at the California Institute of Technology in Pasadena. There he quickly encountered smog. He says it was an "obvious choice" for him to work on air pollution, and he has been developing pollution models for more than 10 years. In 1984 he went to teach at Carnegie Mellon.

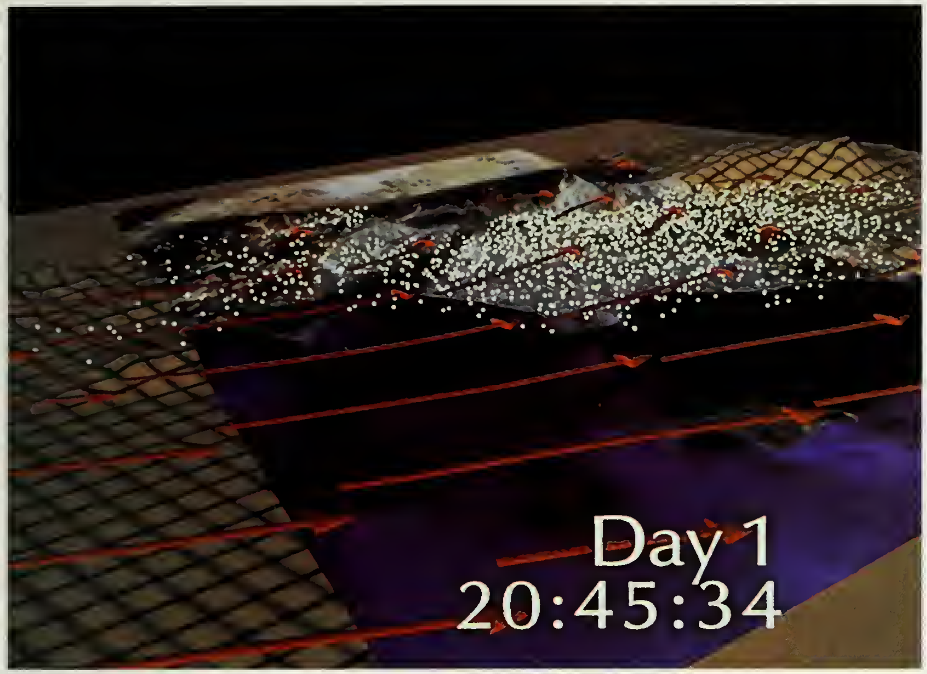


Still from smog video showing concentration of LA's ozone (orange) and carbon monoxide (green) on Day 2 of a three-day period. The red line in the bar graph indicates the federal acceptable standard. (Courtesy NCSA Visualization Services and Development group.)

McRae has been using the data-crunching power of high-performance computers at the Pittsburgh Supercomputing Center (PSC) to run complex models of ozone and other pollutants. His skills learned on the X-MP have rapidly transferred to PSC's latest machines—currently the Y-MP and a Connection Machine.

McRae's computer modeling of large atmospheric systems caught the attention of the Society for Industrial and Applied Mathematics (SIAM). At the Supercomputing '89 Conference in Reno last November, the society granted McRae their Forefronts in Computational Science award for his unique contribution to computational science in modeling large atmospheric systems on the computer.

Working with Armistead Russell, a mechanical engineer at Carnegie Mellon, McRae developed an atmospheric model of the LA basin that takes into account rates of emission of pollutants, their changing chemistry, and the effects of wind and weather. To show how these conditions cause the formation and movement of ozone and other pollutants, McRae and Russell produced two-dimensional contour maps of the LA area.



Still showing dispersal of pollutants by wind in LA basin (Day 1 of the same period as the previous view). Each white ball equals 10 metric tons of nitrous oxide. (Courtesy NCSA Visualization Services and Development group.)

McRae says their work has had a major impact on public policy. In 1988 and 1989, their research provided a scientific foundation for the comprehensive Air Quality Management Plan in the Los Angeles Air Basin. And more recently, McRae said the NCSA-produced visualization will play an important role in the California State Implementation Plan for controlling air pollution.

Early this year in an interview with *PSC News* (Pittsburgh Supercomputing Center's newsletter), McRae said that to effect changes in public policy, researchers need to communicate to people not trained in the sciences. Using high-performance computing to obtain calculations is largely irrelevant to a U.S. Senate hearing, according to McRae. But he stated that "visualization is extraordinarily important" for conveying information produced on the supercomputer.

McRae said it would be difficult to single out one video as having affected overall policy change on pollution control, but he cited a case in which his research has changed policy. His work persuaded the EPA to adopt more stringent controls on air-polluting nitrogen oxides. McRae used preliminary versions of the NCSA visualization when he testified before the Southern California Air Quality Board last December, but he said it is too early to tell the impact on policy from this latest visualization.

"State and local agencies are very enthusiastic about the use of visualization tools—not only for unraveling the physics and chemistry that's occurring," he adds, "but also in providing a way to educate the general population about the complexity of air pollution problems and the need for controls."

Collaborating at NCSA

Last December McRae spoke on his research in the Cray Supercomputing Seminar Series at the Beckman Institute [see ***access***, February 1990]. While at NCSA, he saw NCSA Research Scientist Bob Wilhelmson's thunderstorm visualization [see ***access***, January 1990]. Calling it "a spectacular piece of work," he wanted his air pollution models visualized with NCSA's techniques. As a result, he began working with McNeill and Sherman in the VSD group.

McRae said his research at PSC and his work with the VSD group at NCSA represents an important collaboration between the centers.

Air pollution *continued on page 20*

Tracking a visualization project

access interviewed William Sherman and Michael McNeill, scientific animators in NCSA's Visualization Services and Development (VSD) group, to describe how Gregory McRae's animation project, "Smog: Visualizing the Components," moved through VSD's visualization process.

Early this year McRae brought Cray-generated data from his pollution simulation and Landsat photographic data for the Los Angeles area on cartridge tape to NCSA. Later, he sent meteorological data and emissions measurements electronically from Pittsburgh via the Internet network.

Since scientific data is received in various formats, first it must be put into a form that can be used by the software at NCSA. The animators wrote custom software to meld McRae's data with existing programs. NCSA's Hierarchical Data Format (HDF), developed by NCSA's Software Tools Group, was used to process and store the data.

McRae's data had previously been visualized in two-dimensional form. On his first day with VSD, McRae worked with Sherman and scientific animator Mark Bajuk, who put together a sample visualization showing a three-dimensional representation of McRae's data. From this they produced a set of stills for McRae to evaluate.

After discussions with McRae, Sherman made a preliminary video of animated images. Sherman worked with Landsat photographic data, which provides a picture of geography in the LA area that could be incorporated into the video images. He converted the Landsat data to a texture file; this gave color to surface features, such as highways.

McNeill joined Sherman sometime later to continue the project. In addition to the Landsat data, they obtained the topographic data for LA and combined this information to produce a three-dimensional model of the area. Meteorological data, such as wind speeds and directions, was also incorporated into the visualization.

Visualizing McRae's data required some programming ingenuity. "The main problem was getting things

Tracking *continued on page 6*

Tracking continued from page 5

registered properly," said McNeill, explaining that he and Sherman had to position three datasets and modify existing programs to handle the data. At McNeill's suggestion, Sherman modified the Integrate code—a VSD-developed program for integrating particle trajectories in a vector field—to utilize the changing emissions data and depict the release of source pollutants (represented as particles) into the atmosphere. In conjunction with Integrate, they used a program called Tracer, written by VSD project leader Matt Arrott, to produce streamlines of wind flow.

Next the animators assigned geometric objects to various data. For example, they chose arrows to represent wind streamlines and spheres for particles of pollution. Then the animators refined colors and textures: they decided to make arrows red and clouds transparent. As they composed each scene, they set up objects in ways that accent interesting features. The animators exaggerated heights by a factor of five to dramatize elevation differences.

Aliza Corson, VSD scientific animator, joined the effort to assist with motion scripting. In planning the motion dynamics of each scene, the animators considered how an imaginary camera would move through scenes and from what angle and direction a viewer could best observe the setting.

Next a shell script was written to generate each frame of the visualization. Software developed inhouse and running on VSD's Silicon Graphics 240/GTX was used to produce four frames in parallel and store completed images. Using Wavefront Technologies software, images were rendered.

After computing hundreds of frames, the images were fed into the editing environment to an Abekas digital disk recorder. Images were recorded one frame at a time and then played back at various speeds. The editing of the animated images—along with titles, credits, and narration—was performed by VSD's Media Services division in coordination with the animators. Bob Patterson, Media Services postproduction supervisor, edited the final videotape, which runs about 2 minutes. ▲

Clouds and the greenhouse effect

by Joseph Hardin, Manager, Software Tools Group

Mathematical models are only as good as their input—especially their underlying physics. And in the case of global circulation models that are being used to predict potential greenhouse effects, some input could be a lot better.

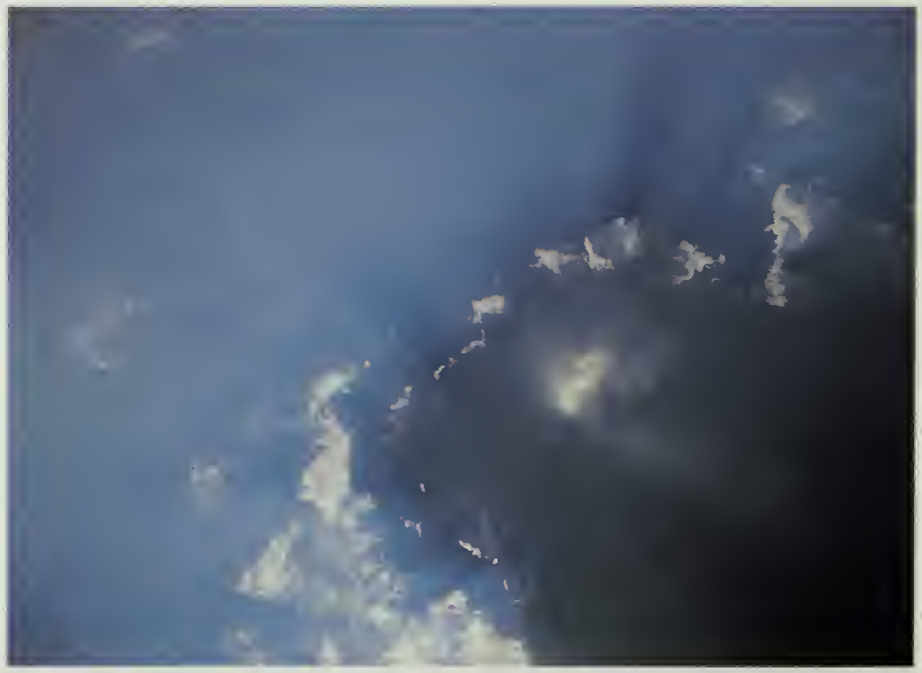
"Currently number one on everyone's list of uncertainties in these projections for the magnitude of the greenhouse warming is the effect of cloudiness," says Phil Austin of Vancouver, BC. "Clouds occur on a small scale and are difficult to put into these global models. So the objective of this research is to learn more about cloud properties—what makes clouds appear and disappear, how much sunlight they reflect, and how much heat they emit back to earth."

"A 'back of the envelope' calculation shows that if the area of low clouds covering the oceans increased by 4%, then that change in the reflectivity of sunlight alone might be enough to counteract the projected greenhouse warming. So small changes in these clouds make for large changes in the amount of radiation that reaches the earth—at both long and short wavelengths. We just don't know enough about them."

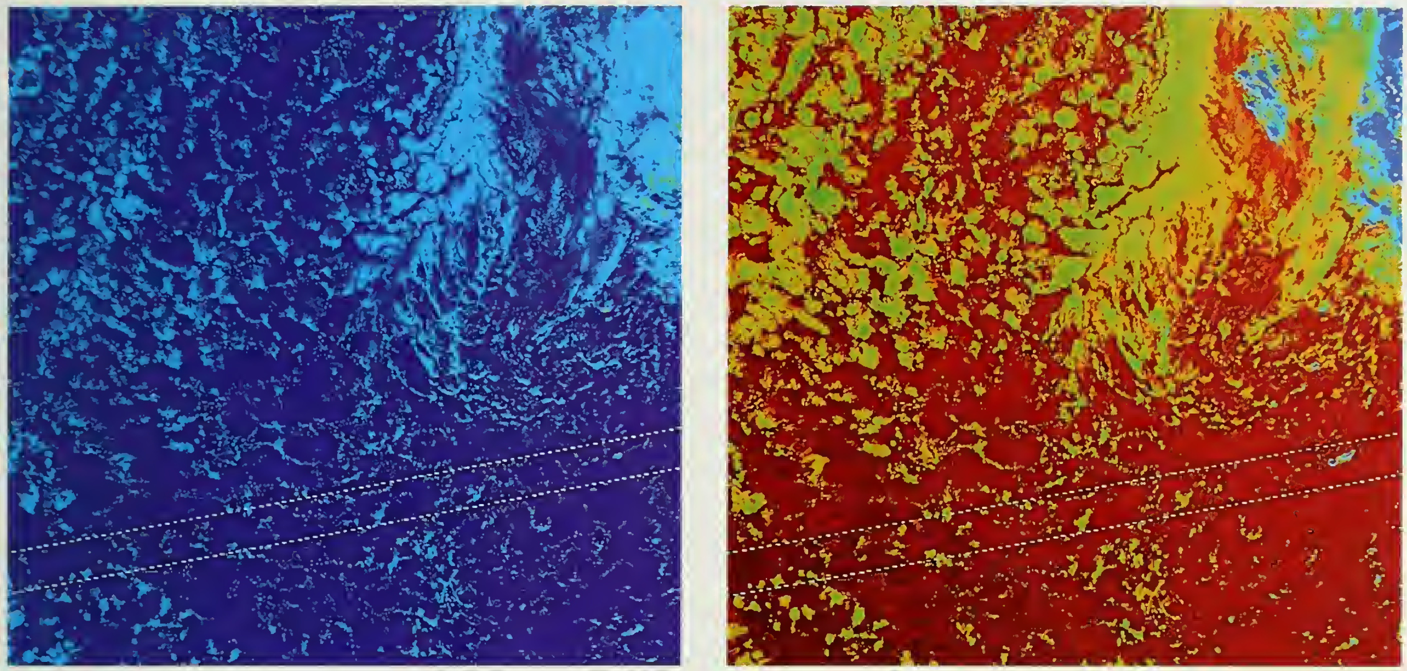
The difference that low clouds make in model projections of global warming is proving to be substantial, since the sensitivity of the models to cloud optical characteristics is high. Builders of the models need to know how these clouds behave in the real atmosphere and how they might respond to a changing climate.

Interpreting satellite images

Phil Austin is a researcher at the University of British Columbia who participates in a large program managed by the National Aeronautics and Space Administration called the International Satellite Cloud Climatology Project Program (ISCCP). The Office of Naval Research and NSF are also major contributors to ISCCP. An assistant professor in the Atmospheric



Stratocumulus (low) clouds over Illinois. (Photo by © David Riecks.)



Satellite images of marine stratocumulus clouds off the California coast on January 5, 1990 viewed with NCSA Image. Channel 1 (left) senses light reflected by the sea surface and clouds at 0.58–0.68 microns, roughly corresponding to the naked eye. Channel 4 (right) is an infrared view of the same scene measuring the temperature of the ocean and the clouds at 3.7 microns. This view shows the tendency for stratocumulus clouds to organize themselves in rings. In both views, land in the upper right can be seen under cold *cirrus* (high) clouds; dotted lines from left to right denote missing data. (Images by the Advanced Very High Resolution Radiometer aboard National Oceanic and Atmospheric Administration satellite, NOAA 10; courtesy Phil Austin.)

Science Program in the Department of Geography, Austin teaches and does research in atmospheric physics, boundary layer meteorology, and remote sensing. His research involves trying to observe and understand the processes that control cloud formation, dissipation, and cloud reflectivity in the real atmosphere—with the hope of finding simple ways to represent these processes in atmospheric models.

Austin currently focuses on interpreting satellite images of clouds. Working with satellite data is a recent departure for Austin, who considers himself to be a boundary layer meteorologist. According to him, a major question for researchers right now is: How do you observe clouds with satellites? "You're always guessing when you look at satellite information," he explains. "There's not enough information reaching the satellite to give you a full description of the cloud layer." Researchers have been struggling to interpret satellite data and to correlate that effectively with the interesting characteristics of clouds being observed. "Twenty years of work have set the stage for this," Austin adds.

"So to answer some of these questions, they launched a series of 'experiments'," he says. The first was for low clouds off the coast of San Diego in 1987. (There are four total: two [Wisconsin and Kansas] for high, *cirrus* and two [San Diego and the Azores] for low, *stratocumulus*.) "The idea was—while satellites were monitoring the clouds—to get aircraft in and above the clouds to compare what the satellites were seeing with what the clouds actually were. That was a joint effort." Three U.S. aircraft participated: a NASA U2Q (called an ER2Q) flew at the top of the troposphere while aircraft from the National Center for Atmospheric Research and the University of Washington and another aircraft from the British Meteorological Office flew in the lower atmosphere. "They flew coordinated patterns inside the clouds measuring radiative fields, cloud droplets, temperature, and turbulence," Austin adds. "An extensive set of surface-based measurements were also collected from instruments on San Nicolas Island."

"Now we're trying to integrate all that information and use the measurements in the clouds to constrain the satellite data. So now, when we monitor the earth over the next 10 years without airplanes—because that's prohibitively expensive—we know what we're seeing when we look at a satellite image."

Measuring water droplets

"One of the things that is a major concern is how big are the drops of water that go to make up a cloud," continues Austin. This tells a lot about how much light the cloud will reflect and hence how much energy will be kept from reaching the earth's surface.

"If you think about a heavy rain cloud, it looks black because there are a few large droplets in that cloud. And the droplets are absorbing some of the radiation. If you think about a puffy fair-weather cloud, it looks bright and that's because there are zillions of brilliant, light-scattering, tiny droplets in there. The difference between the dark cloud and the bright cloud is very important to the amount of radiation that's reaching the ground."

Austin explains that the combination of satellite data and airplane fly-through can be immensely helpful. "For instance, there's one channel (from the satellite data) at 3 microns," he says, "in which the reflectivity is different if there are large droplets or small droplets. In addition, the visible channel is brighter if the clouds are thick than if they're thin.

Clouds *continued on page 19*

FMC quickens the pace

by Kathleen Robinson, Science Writer

As a recently joined NCSA industrial partner, FMC got off to a running start with nine Cray projects well underway in six months and ten more projects in the planning stages. Nevertheless, some members of the FMC management team finished a recent workshop convinced by NCSA Director Larry Smarr that their researchers could be using NCSA's facilities even more. After an industry overview presented by Carl Diem, director of Marketing and Benchmarking at Cray Research, Inc. (CRI), at least some of the FMC managers thought that their company may have entered the supercomputing partnership just in time.

In the first part of their two-day meeting at NCSA in May, research managers from across FMC were bombarded with projections about the next few years of supercomputer development and applications. Smarr showed graphics depicting the exponential growth—both in hardware and software—of supercomputer power. Pointing out the historical pattern of a tenfold increase in capability every 3 years, he said, "This means that it costs a factor of 10 less every 3 years to do the same job. If you're going to be spending the same kind of money, you'd better be figuring out how to do something ten times as hard, every 3 years."

Setting expectations

FMC has recognized "that the *management* of technology is at least as important as its use by researchers," Smarr said as he applauded FMC's vision in arranging this workshop for managers from across the corporation. He spoke of the need to keep managerial expectations in line with reality. "Some people assume that anything thrown onto a supercomputer will run fast. That simply will not happen, in some cases—even if you optimize the code. The inherent nature of the algorithms—the inherent nature of the physics that you're trying to solve—will give a wide range within your corporation to a set of application codes. In terms of management, it is very important that your expectations be set by what the technology can deliver. And if you've got a problem that's going to take *man-years* to attack, you should rethink the way the code is written to take advantage of vectors and multiprocessors that will be available soon."

To meet this challenge, Smarr added, NCSA is hoping to pull together faculty from computer science and engineering that will help NCSA work on algorithms for its application areas.

FMC managers tour NCSA's visualization facilities under the guidance of Steve Pruiett-Lane, scientific visualization animation producer (right). (Credit Vincent Jurgens, NCSA Media Services.)

Going through the roof

In another presentation, Carl Diem from CRI showed example after example from industrial applications where "the size and complexity of problems have just been going through the roof. To keep the response time reasonable, you really need the biggest machines." One example was "an interesting little electromagnetics research problem, [that] took 17 elapsed hours on an eight-processor Y-MP with all eight heads running."

His most extreme example was a project scientists at NCAR would like to be able to do. A thousand-year oceanographic study, he said, "that would require 3.5 years of X-MP/48 clock time per year of the study. That's not going to get the job done! If they did have a teraflop machine, that would take 27 hours of wall-clock time per study year. So it's clear," he concluded tongue-in-cheek, "that we [supercomputer manufacturers] are the bad guys—we're standing in the way of scientific progress."

Diem showed examples of Cray usage from industries all over the world, including some possible FMC competitors. (With a chemical and machinery product line that ranges—alphabetically, at least—from aeration equipment to zinc oxide, FMC could face lots of competition.) Diem sketched a dire scenario for companies that have not turned to supercomputers for their R&D.

Workshop sessions

The first afternoon session was a presentation from Donna Cox, associate director of education for NCSA and UIUC associate professor of art, explaining the concept of "Renaissance teams" that she developed. Now that the breadth of knowledge makes generalization unfeasible, according to Cox, the need for teamwork among talented professionals from diverse fields is becoming more and more clear.

Cox was followed by Dan Brady, manager of Visualization Services and Development. FMC used this group's expertise for a project soon after affiliating with NCSA. Brady explained various levels of support the group provides, and the stages involved in projects such as ones FMC has done.

The second day of the workshop consisted of two concurrent morning sessions. A workshop on chemical applications was cochaired by NCSA Research Scientist Harrell Sellers and Gerald Gruber, FMC chemical engineering specialist. Greg Clifford, manager of Engineering Applications at CRI; M. Fouad Ahmad, visiting research scientist at NCSA; and Ramesh Jayaraman, NCSA computational fluid dynamics project leader, conducted a session on engineering applications. Clifford gave a presentation on CRI's engineering applications.

Thinking strategically

One of the FMC participants was John Luranc, director of Manufacturing and Engineering Computing. He described his role, and that of other managers at the workshop, as one of being "missionaries, so to speak, charged to take the message back home" with them.

The *message* being that high-performance computing is unlike any technology ever known—not only in terms of its potential for enabling R&D, but also in its relentless forward pace. There is no time to pause—companies that will dominate the marketplace in the future are those developing a strategic relationship with supercomputing. ▲

A pioneer returns home

by Jarrett Cohen, Public Information Specialist

Larry Ray, Eastman Kodak Co.'s on-site partner representative since 1986, was recently transferred back to the company's headquarters in Rochester, NY. Ray will continue to be an NCSA user—employing high-performance computing to optimize various electronic imaging processes in Kodak's Electronic Imaging Division.

In tribute to Ray's dedication and contribution to computational science and visualization, ***access*** interviewed him about his recollections of the NCSA-Kodak partnership.

NCSA's first industrial partner

Ray had only been at Kodak for about 2 years when he had his first contact with NCSA Director Larry Smarr at a Cray Research, Inc. symposium in 1985. "I heard him concoct the idea of an industrial program," said Ray, which immediately excited him. "We were looking for ways of introducing Kodak's scientific and engineering community to supercomputing as well as trying to find out if the company needed supercomputing at all," Ray added.

Smarr's speech at the CRI symposium and a subsequent conversation convinced Ray, and in turn his superiors at Kodak, to look at the NSF centers. "Illinois was one of the prime candidates," Ray explained, "as NCSA seemed to be closest to the model of a successful academic-industrial partnership."

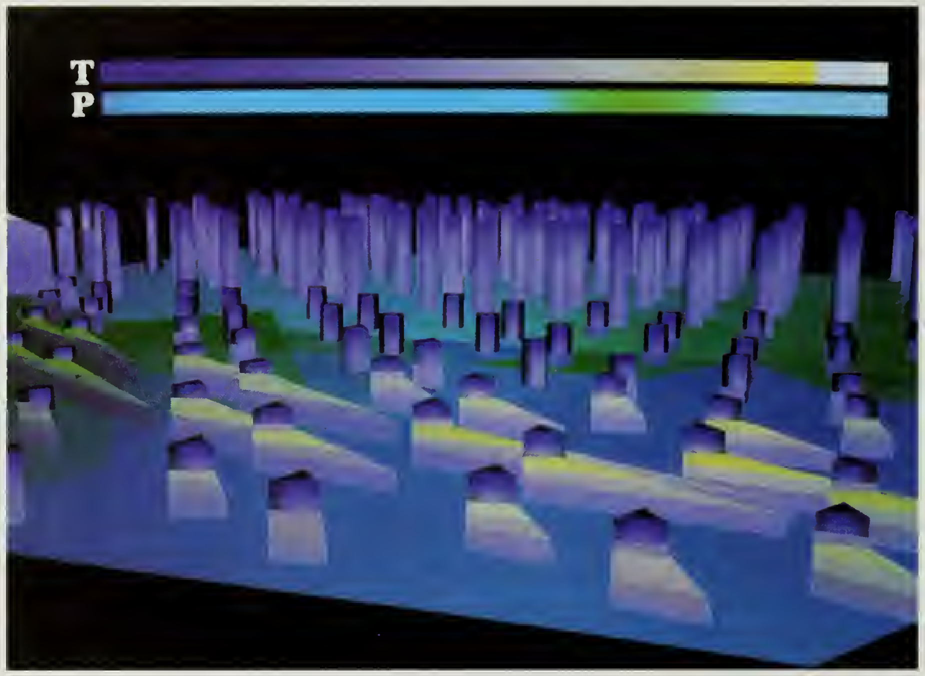
In November 1985 Ray, then a Kodak research scientist; Edwin Przybylowicz, Kodak senior vice president and director of research; and about seven division directors flew out to Champaign by corporate jet. This group formed the first industrial visit to NCSA.

All were immediately impressed, despite NCSA's small size—only about 10 full-time staff—at the time. Indeed, Ray described Przybylowicz's response as "not *if* we would do this but *how* we should do this." Next was the matter of getting corporate support for becoming an industrial partner, which Ray said was difficult at first; eventually Ray and his supporters succeeded.

Pioneer *continued on page 10*

John Stevenson (left), associate director of the Industrial Program, presents Julie and Larry Ray (right) a poster of "The Worm Race" as a farewell gift. Mary Helen Waters, secretary to the Industrial Program, looks on (center background). (Credit Cordelia Baron, NCSA Media Services.)

Simulation of the flow of molten plastic inside a steel mold from NCSA–Eastman Kodak animation, "Plastic Injection Molding." (Credit Rich Ellson, Eastman Kodak; Donna Cox and Ray Idaszak, NCSA.)



***Pioneer** continued from page 9*

"We were getting serious here and had to get into writing a contract," Ray said. "I talked to Jan Wehmer [long-time assistant to Smarr] and asked for a sample contract. There was a pause on the line. We had to write one from scratch!"

After a period of negotiating, the contract was signed in May 1986, and Kodak became NCSA's first Industrial Partner.

Early days at NCSA

Ray returned to NCSA in August 1986 as a senior research scientist and Kodak's on-site partner representative. The latter position created something of a tradition in the Industrial Program, with most of the six partners to follow having on-site representatives as well.

"It was very exciting around here," Ray said. "Good things were going to happen at NCSA and at Kodak."

Soon after Ray's arrival, he was joined by a second Kodak researcher, engineer Ron Auble. Auble produced, along with NCSA consultant Dave Heisterberg (now at the Ohio Supercomputer Center), the first Kodak visualization videotape. It depicted heat transfer in an optical disk that occurs as a laser beam transits a region.

"It was commonly known as 'The Worm Race' because of the layers of heat traveling across the screen," Ray stated. "As the layers had different temperatures because of the thermal diffusion, it appeared as if a race among ten contestants was occurring."

The tape took about three weeks to produce. Today it would take less than a day, and "we would have better graphics," Ray said.

Strides in visualization

"The Worm Race" began a series of visualization projects that broke new ground in several application areas of importance to Kodak. Ray listed these: designing headlight reflectors, fluid dynamics in film manufacturing, surface chemistry and catalysis, and various chemical and manufacturing processes.

According to Ray, Kodak's greatest success at NCSA was the plastic injection molding project. In simulating this complex engineering process on the Cray, Ray's team soon came to grips with the underlying physics of the problem. The project was undertaken by engineer Richard Ellson, who came to NCSA in 1987 and returned to Rochester in 1989. Collaborating with Ellson in what has come to be called a "Renaissance team" were NCSA's Donna Cox, artist, and Ray Idaszak, visualization specialist. The team used triangular glyphs to represent pressure, temperature, and velocity—key variables associated with the process. Shape indicated velocity; color scales conveyed pressure and temperature.

In the November 1988 issue of *Simulation*, Ellson and Cox described injection molding as "an economical method for manufacturing thin-walled structures with complicated shapes." They list telephone handsets, cases for video- or audiotapes, ice trays, and slide carousels as items produced by this process.

Visualization of injection molding was first accomplished on a Sun Workstation and was later ported to an AT&T Pixel Machine selected by Kodak, which arrived at NCSA in September 1988. A real-time version of the visualization, currently used on the design floor at Kodak's headquarters, runs on both platforms.

Learning from one another

Ray said that the greatest benefit of the partnership has been in becoming sophisticated about understanding high-performance computing—particularly visualization. "I would like to think that we have contributed to that whole genre," he said.

John Stevenson, associate director for the Industrial Program, added that NCSA has greatly benefited as well. "There has been a lot of sharing, and NCSA has learned a lot about corporations through Kodak's participation," he said. "I have the highest regard for Larry and his family. He became more than a corporate representative; he became part of the team."

In the closing moments of his interview, Ray expressed a similar sentiment: "It has been an exciting four years here. I would not have passed it up for anything. I have gained more than I have ever given back." ▲

Reinventing partnerships for the '90s

Industrial partners executives pose with NCSA's directorial staff and Industrial Program directorial representatives at the annual NCSA Industrial Partners Executive meeting. Industrial partners attending included Amoco, Caterpillar, Dow, FMC, Eli Lilly, Motorola, and AT&T. NCSA Director Larry Smarr spoke to the group about high-performance computing, industrial competitiveness, education, and the environment. (Photo by Wilmer Zehr.)

Education

Supercomputing and undergrad physics

By Kathleen Robinson, Science Writer

"After I was here last year I was able to go back to campus, write up a lab exercise that used color graphics interactively, and within just weeks my students were using it. That was their favorite lab." Amy Bug, assistant professor of physics at Swarthmore College, came to NCSA last summer as a participant in the Workshop on Supercomputer Education presented by Nora Sabelli.

Located in Pennsylvania, Swarthmore College is a member of NCSA's Academic Affiliates Program where Bug is institutional representative.

For a week this spring, Bug returned with NSF funding provided by NCSA to develop a series of modules that use high-performance computing to teach computational physics concepts and scientific programming techniques to undergraduates—in a format suitable for widespread dissemination.

"There's a big difference between giving students a scientific package to use and letting them experience programming for science," says Bug. "The former is not time-intensive, but it's not very instructive, either. Having students do the programming is very instructive but also very time-intensive. Unfortunately, most departments are already struggling with an overcrowded undergraduate syllabus and can't afford to give much time to any one topic. We have to try to find a middle ground."

Designing the project

Bug and another Swarthmore physicist, John Boccio (Swarthmore's assistant provost for academic computing), describe their project as a minicurriculum that could either be pursued by an individual undergraduate science student as a special project or be included as part of a full course on computational methods. The project will include student tutorials plus model codes and results for instructors.

An instructor with little previous experience in supercomputing should be able to use the modules, according to Bug. Topics will include Monte Carlo integration of functions of single and multiple variables, Metropolis Monte Carlo applications, and the generation of random variables. Techniques to be stressed will be vectorization, parallelization, and optimization of code.

Perhaps the most difficult part of the project is finding a way to design exercises that can be used on a number of machines with a range of software packages while making the attributes of various machines and packages part of the curriculum. The approach proposed by the Swarthmore team is to present algorithms rather than programs and to use the most generic versions of machines and protocols.

Involving an undergraduate

Swarthmore College has a tradition of involving students in the design and administration of their education and that tradition continues with this project. Undergraduate student Eric Stollnitz, who just completed his sophomore year, received NCSA support that enabled him to come to NCSA with Bug. One of two recipients

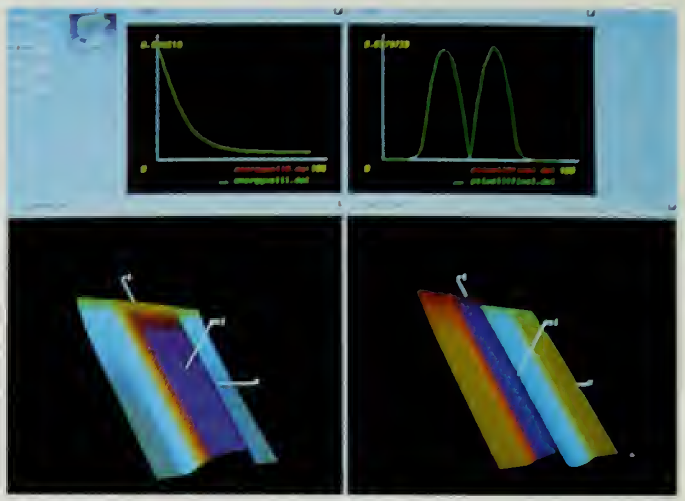
***Undergrad physics** continued on page 12*

***Undergrad physics** continued from page 11*

of the Goldwater Fellowship from his home area of DC, Stollnitz worked hard at writing and debugging three different codes from scratch in a week.

"We came with no written code at all—just ideas based on other codes we had written," says Bug. "And the idea was for us to be the students—for us to write the codes, debug them, and optimize them. Being *here* at this point in the project helps a lot, because we can just walk down the hall and get help from NCSA staff like David Ceperley, who has been very helpful. Then we'll go back home and work on the tutorials and the instructor package." In future, Bug plans to present her results at a conference on teaching physics.

Also accompanying Bug this year was her youngest student yet—Murphy Reshard Bug, age 3 months. Seated on his mother's lap before an IRIS in the Renaissance Education Laboratory, he seemed perfectly at home. Commented one observer, "The researchers are getting younger every year!" ▲



Employing a quantum Monte Carlo method to find the wave function of a particle in an arbitrary potential, Bug and Stollnitz generated this graphic with the CRAY X-MP/48 and NCSA-produced software. Evolution from a random initial state to the correct wave function is shown. (Courtesy Amy Bug.)

CS&E education workshop: call for ideas

by Nora Sabelli, Senior Research Scientist

Although the effect of computational science and engineering (CS&E) on research has led to many programs to expand high-performance computing access and use, there is no comparable understanding of how to transfer the enabling effects of this technology to the field of education—particularly at the precollege level when students are developing career choices and attitudes about science and engineering.

The NSF-sponsored supercomputing centers are in an ideal position not only to catalyze the transfer of CS&E tools, techniques, and experience to the educational community, but also to help educators prototype for the future. The four NSF-funded supercomputing centers will convene and host a two-day panel session to discuss educational issues, analyze data, and make recommendations at a workshop to be held October 28–31. Panel discussants will explore ways that CS&E can make contributions to enhance education for students at precollege, college, and university levels.

Dates for the workshop have been chosen to allow time for a presentation of the panel's recommendations during Supercomputing '90, November 12–16, New York City. Educators and their institutions, high-performance computing centers, and funding bodies comprise the target audiences for the panel's recommendations.

Topics for discussion include the following:

- How can the NSF-sponsored centers support student/teacher access to advanced scientific computing?
- How can the centers promote teacher familiarity with and skills in using computational tools?
- When is the best time to introduce high-performance computing into the curriculum?
- What should be done at each educational level?

The focus will be on involving students, teachers, and administrators with vendors and technology while the infrastructure for delivery is being put into place.

It is anticipated that the group will confront what supercomputing centers can contribute to math and science education at the precollege and undergraduate levels; provide answers to how today's desktop technology can be used by students and teachers; provide examples of existing programs that can be emulated and built on; and distribute multmedia materials—such as videotapes of visualizing scientific concepts, Hypercard stacks, and CD-ROMs—to educators afterwards.

Final announcements about the agenda and selection of panelists will be made by the Steering Committee. The NSF Divisions of Advanced Scientific Computing (Computer Information Sciences and Engineering) and Teacher Preparation and Enhancement (Education and Human Resources) are sponsoring the panel.

If you would like to be considered for membership on the panel or collaboration on its studies, contact Nora Sabelli, senior research scientist and Educational Outreach contact [see **NCSA contacts**, page 23]. ▲

Equipment loan for elementary education

by Jarrett Cohen, Public Information Specialist

Three Champaign-Urbana elementary schools recently received $50,000 in computer equipment and special software in a model program to stimulate math and science education. NCSA and UIUC's Computing Services Office (CSO) jointly sponsored the equipment loan to Dr. Howard and Robeson Schools in Champaign and Leal School in Urbana.

"Part of NCSA's mission is to educate, empower, and inspire teachers and students in the elementary grades to develop an awareness of and an interest in science and mathematics," said Scott Lathrop, associate director for NCSA's Academic Program and coordinator of the project. "We are providing the tools, information, and support to enable teachers to expand their educational capabilities."

Among the speakers at the mid-May dedication held at Dr. Howard School were Rob Wolff, senior scientist at Apple Computer, Inc.; Timothy Hyland, Champaign superintendent of schools; Richard Bodine, principal of Leal School; and Larry Smarr, director of NCSA.

"This is the first time I've really understood the depth to which our technology can help [the educational] process," said Wolff. "This is just remarkable. We are hoping to expand the program next year and to have the capabilities of students doing real-time simulation. . . . We are consulting and working closely with the people at NCSA."

Transferring technology

Equipment loaned includes two Macintosh IIcx systems, 14 Macintosh Plus systems, two LaserWriter printers, and an AppleTalk network to interconnect the systems at each school. In addition, Champaign Unit 4 school district plans to connect the computers at Dr. Howard and Robeson by modem for collaborative science projects. "The Macintosh equipment will give us an opportunity to explore the use of emerging technologies with younger students in a collaborative setting," said Sue Zellers, director of Educational Technology, Champaign school district.

The computers were equipped with NCSA-developed scientific software tools plus traditional word-processing and drawing software. NCSA hopes to learn how to better develop its software tools for elementary schools. Center researchers will observe how students use the new resources and will work with all local schools to build upon the program with new proposals to funding agencies and computer companies.

Part of a national movement

Smarr sees the loan as "NCSA and CSO's part in a national upsurge of concern about K–12 education"—a concern that reaches the highest levels of the federal government. D. Allan Bromley, President Bush's science advisor, has told Congress that by the year 2010, all U.S. elementary and high schools should join the nation's major universities, laboratories, and research-oriented corporations on the National Research and Education Network (NREN), a fiber-optic information "superhighway." AT&T research scientist Michael Condry, with whom NCSA has been researching networking, will study the three schools' opportunities in this area.

Teachers at the three local schools began training in mid-April with NCSA's assistance. The computers will be used by children in grades 4 and 5 at Dr. Howard and Robeson, and in grades 3 through 6 at Leal. ▲

Rob Wolff, senior scientist at Apple Computer, Inc., spoke at the computer equipment dedication.

Students got acquainted with the Macs at the open house that followed. (Credit Cordelia Baron, NCSA Media Services.)

Charlie Reiman earns NCSA scholarship

by John Melchi, Public Information Intern

Charles Reiman. (Photo by John Melchi.)

Charlie Reiman received the 1990 NCSA Undergraduate Employee Scholarship Award for his continuing efforts in developing a switched, 56 Kbps (Kilobits per second) network interface to the Apple Macintosh system. He is a programmer in the Networking and Systems Development Group.

"I was giddy," Reiman laughed. "I felt like I had won a game show."

Reiman is majoring in computer engineering at UIUC and expects to graduate in May 1992. NCSA established the Undergraduate Employee Scholarship Award in 1988 to acknowledge outstanding efforts by an undergraduate staff member. The award provides tuition for one year at UIUC.

In June 1989, his first summer at NCSA, Reiman wrote a complex network management and monitoring system and showed excellent programming skills, says Charlie Catlett, Networking and Systems Development Group manager. Since then, he has been working on an AT&T-funded project building an innovative, switched, 56 Kbps network interface to the Macintosh.

"Usually, when you use a 56 Kbps line or a high-speed digital line, you lease it and pay for it 24 hours a day, 30 days a month, all of the time. It is a dedicated line," Reiman said. The goal of the AT&T project is to design a switched, 56 Kbps line that will allow the user to only pay for actual time on the network rather than for continuous service.

New capabilities

"This just isn't being done, typically," says research programmer Gary Faulkner, with an enthusiastic grin. "This is a new capability. It is not something that people can do today. It is not new technology, because switched lines have been around for awhile; 56 Kbps lines and NCSA Telnet have also been around for awhile. It is putting all of these things together that has never been done before."

The switched line will provide high-speed access at remote locations—even to researchers not directly connected to NSFNET. Reiman took the initiative to communicate with Apple Computer, Inc. and successfully obtained $3,000 worth of donated hardware and software.

"We have been quite fortunate, because we certainly didn't have anybody else here on our staff who could have done what Charlie is doing," says Faulkner. "He has a good Apple background, and that is going to make it a lot easier for us to get ahead working on the Macs."

Playing a vital role

Catlett also pointed out the vital role Reiman holds in the Networking and Systems Development Group. "His contribution to the group and to NCSA, however, goes far beyond programming skills. He is also responsible for keeping our staff Macintosh systems up to date with a uniform software suite, bug fixes, and system enhancements. Further, he ensures that all of the group Macintosh systems are backed up according to a regular schedule."

Previous recipients of the NCSA Undergraduate Employee Scholarship Award are Gaige Paulsen, 1988 [see ***access***, September–October 1988], and Dave Thompson, 1989 [see ***access***, November–December 1989]—both of whom have worked in the Software Tools Group. ▲

NCSA participates in SIGGRAPH '90

NCSA will be making its mark on ACM's SIGGRAPH '90 program with involvement in panels, visual presentations, seminar presentations, and a software demonstration. This year's meeting will be held in Dallas, TX, August 6–10.

NCSA Director Larry Smarr will chair a panel entitled "Grand Challenges of Computational Science." Panelists will explain visualization's role in tackling the U.S. government–mandated challenges at university, industrial, and government research centers. The White House's High-Performance Computing Program will also be discussed. Panel members will be Gregory McRae, Carnegie Mellon University; Arthur Freeman, Northwestern University; David Dixon, E. I. Du Pont De Nemours & Co.; and Eric Lander, MIT.

Cox to fill many roles

Associate Director for Education Donna Cox will be participating in the conference in a variety of roles. First, Cox will be chairing two panels. For the panel on "Beyond Scientific Visualization: Mapping Information," Cox will present NCSA's visualizations and techniques in mapping information. Researchers participating in the panel will be Richard Ellson, Eastman Kodak Co.; Helga M. Leonhardt Hendriks, The Leonhardt Language System; and Jim Blinn, California Institute of Technology.

Members of the panel "What Is Happening on the Hill?" will address how federal policies impact research in computer graphics. Speakers will include Smarr; Jacob Maizel, Jr., National Institutes of Health; and Rich Hirsh, National Science Foundation.

Also a UIUC associate professor of Art and Design, Cox and members of her Visualization Experimental Technologies class (a collaborative workshop in computer animation) will present an animation entitled "Venus and Milo" that will be shown in the Animation Screening Room. Bob Patterson, NCSA Media Services post-production supervisor, edited the animation; music was composed by Robin Bargar, UIUC graduate student in music.

Cox was recently reelected to a second term on SIGGRAPH's Board of Directors.

NCSA presentations

Matthew Arrott, project leader in NCSA's Visualization Services and Development (VSD) group, will present a paper entitled "Communication as It Pertains to Scientific Visualization" in the State of the Art in Data Visualization course. Mike Folk, senior programmer in NCSA's Software Tools Group (STG) will be presenting "HDF Vset" in the workshop on "Data Structures and Access Software for Scientific Visualization." Jason Ng, NCSA senior programmer, coauthored the paper.

STG will be showing NCSA-produced visualization software in the Apple Computer, Inc. exhibition. Brian Calvert, Ron Mabbitt, and Dave Thompson will be demonstrating the software.

VSD participants

NCSA's Visualization Services and Development group (VSD) recently got word that a number of their presentations and productions are to be part the conference. Members of VSD and their productions involved this year are as follows:

Film and video show

"Computational Quantum Chemistry in Catalysis Research" by Jeffrey Thingvold (visualization); Aileen Alvarado-Swaisgood, Mark Barr, Keith Baumruck, April Swanson, Don Hopkins, Christopher Marshall, and Don Washecheck, [Amoco Oil Co. Research and Development]; Gerry Zajac, [Amoco Corp. Analytical Services]; Jeffrey Tilson and James Harrison, [Michigan State University]; and Harrell Sellers [NCSA] (scientific research); Bob Patterson (editor)

"Landscape Dynamics of Yellowstone Park" by Alan Craig (visualization); David Kovacic , [UIUC]; William Romme, [Fort Lewis College]; and Don Despain, [Yellowstone National Park] (scientific research); Bob Patterson (editor)

"Smog: Visualizing the Components" by Aliza Corson, Michael McNeill, and William Sherman (visualization); Gregory McRae and Ted Russell [Carnegie Mellon University and Pittsburgh Supercomputing Center] (scientific research)

Technical slide set

"Computational Modeling of Insulin Analogs" by William Sherman and Mark Bajuk (visualization); James Metz, James Shields, David Gorenstein, and Claude Jones [Eli Lilly and Co.] (scientific research)

"Energy Density of Higgs Field at the Time of Inflation" by Matthew Arrott and Mark Bajuk (visualization); David Hobill [NCSA], Larry Smarr [NCSA], and David Schramm [Fermilab] (scientific advisors)

"Untitled" by Michael McNeill (visualization); H. R. Chang [Motorola] (scientific research)

Personal participants

Several VSD staff members will be presenting visual productions on a personal basis. Their entries are as follows:

Animation Screening Room

"In Search of the Fingerprints of God" by Mark Bajuk, Matthew Arrott, Jeffrey Thingvold, Jeffery Yost (visualization); Vincent Jurgens (camera); Bob Patterson (editor) *Two Guys from Ohio* by Daniel Boord (producer and director)

Art show

"Pocket Visualization" by Mark Bajuk and Mysoon Rizk

Film and video show

"Under the Puddle" by Aliza Corson (animation); Daniel Remler (music); John Fujii, Susan Amkrant (software); Bob Patterson (editor)

For further information about NCSA at SIGGRAPH '90, see the next edition (September–October) of ***access***. ▲

Molecular dynamics workshop

by Kathleen Robinson, Science Writer

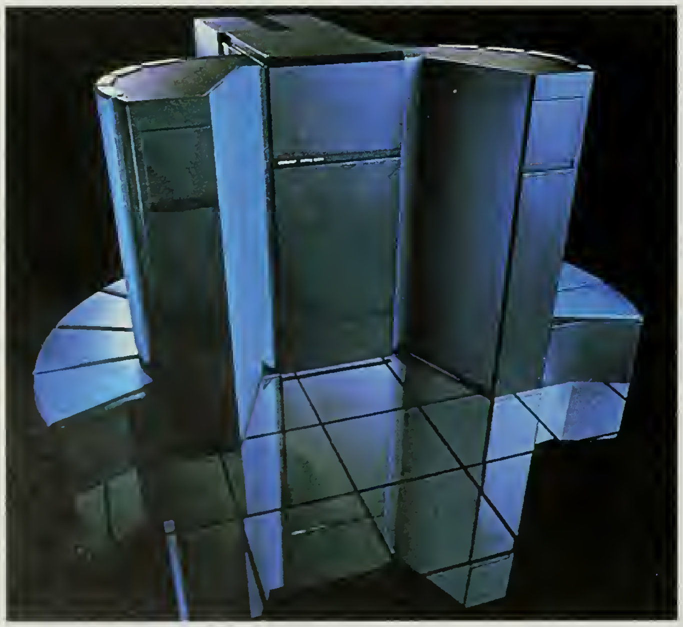
Molecular mechanics...molecular graphics...dynamics simulations... semi-empirical and ab initio quantum mechanical methods. Many of the computational chemists attending a recent five-day workshop were already using more than one of these techniques in their daily research. Consequently workshop discussions quickly went beyond the level of "how-to's" into fundamental issues regarding theoretical and practical difficulties with the techniques, the validity of ab initio calculations, and analysis of the results (which are both voluminous and theoretically problematic).

The 50 participants in the Molecular Dynamics Calculations on High-Performance Computers Workshop [see access, April 1990] represented a broad spectrum—from industry, government labs, colleges, and university research programs. Blending theory and practice proved extremely useful to many of the participating scientists. Randall Kok, assistant professor of chemistry at Milliken University, was able to accomplish "several months' worth" of research, while also meeting more varied users of the techniques than he had known exist. "I'm always looking for ways to make this subject seem relevant to undergraduates," he said. "The people here are good examples of a whole range of applications."

A recurring theme in the evaluations of the workshop was the incalculable value of the sharing—of codes, information, and insight—that took place between participants. The workshop was directed towards research scientists with a basic knowledge of the field who needed to become better acquainted with computational modeling strategies.

Three molecular dynamics software vendors—Biosym, Polygen Corp., and Tripos Associates—participated in the workshop by hosting evening gatherings and by providing overviews and guided walk-throughs of their packages. Their representatives also joined users in frank discussions of the limitations and shortcomings of the current generation of computational chemistry software, and features that would be useful in future versions.

This event was cosponsored by NCSA and the Beckman Institute with partial NSF funding. ▲



CRAY Y-MP4/464. (Courtesy Cray Research, Inc.)

CRAY Y-MP system to be installed

NCSA users will realize more computing power, larger memory, and faster throughput when the CRAY Y-MP 4/464 is installed by mid-October. (The first "4" indicates the maximum number of processors this machine's frame can accommodate; the second, the actual number installed.)

The machine's 64 Mword (megaword) memory will represent an eightfold increase over the X-MP. Its 6-nanosecond clock cycle will make for about 30% faster processing capabilities. Its 128 Mword SSD (solid-state storage device) will solve larger problems that require extensive I/O.

Negotiations have been completed and the purchase has been approved by the Board of Trustees of the University of Illinois. Migration plans for moving to the new system are underway and users will be shipped a Migration Guide in October.

The Y-MP will replace the X-MP while the CRAY-2 will remain at NCSA. And the UNICOS operating system will be utilized as previously. Software for the X-MP can be run on the Y-MP in X-mode without recompiling. Shakedown of the new system is anticipated to be completed within 2 weeks of its installation. Users will be alerted to power-down periods. Potential users of the Y-MP are encouraged to apply for allocations on the new machine.

For further information, watch news and online documentation. If you have questions or comments, contact the Consulting Office [see **NCSA contacts**, page 23]. ▲

Expanding central facilities

Work is well underway to expand NCSA's facilities at the Advanced Computation Building (formerly the Astronomy Building) where the CRAY-2 and the CRAY X-MP/48 are housed. The UIUC Department of Astronomy recently moved into its new quarters which freed up more space for NCSA's Central Facility group and hardware. With this expansion, NCSA will gain another machine room with 4,800 square feet. (Credit Cordelia Baron, NCSA Media Services.)

Networking

NCSA establishes FDDI network testbed

by Charlie Catlett, Manager, Networking and Systems Development

NCSA recently completed a study of internal networking needs for the early 1990s. The purpose of this study was to assess NCSA's current computational infrastructure and to determine how to keep NCSA's facilities at the state-of-the-art. As a result of the study, NCSA's network architecture was targeted for upgrade, a migration path was specified, and high-speed network beta test activities were outlined.

This study measured current network utilization and performance and identified key services, technologies, and limitations in the current network. In-house experts documented current technology, observed trends, and investigated near-future technologies (over the next 12–18 months). The assessment included networks, workstations, distributed applications, visualization software and hardware, storage technologies, and supercomputers.

Several major initiatives resulted from this effort. First, a 100 Mbps (million bits per second) Fiber Distributed Data Interface (FDDI) testbed was installed to evaluate performance and reliability of various products. Second, NCSA joined the American National Standards Institute (ANSI) committee responsible for 800 Mbps HIPPI (High-Performance Parallel Interface), and a representative from NCSA sits on the ANSI committee.

This network update supports today's powerful workstations, NCSA's newest supercomputers—the CRAY-2 and the Connection Machine, and major initiatives in Gigabit per second networking research. These and other activities are aimed at improving the performance of NCSA's computational environment for the typical remote or local user.

Current network architecture

The NCSA network is a collection of 20 Ethernet subnets located in six buildings on the UIUC campus. Ethernet subnets are connected via Internet Protocol (IP) routers and a private NCSA backbone, a Network Systems Corporation (NSC) HYPERchannel-50. UIUC operates a campus network that NCSA uses for a secondary backbone. The campus network consists of Proteon ProNET-80 networks that connect about 75 campus buildings.

The NSFNET backbone node at NCSA is operated by the UIUC Computing Services Office Network Operations Center, which also maintains the campus ProNET networks and various off-campus academic connections, including a CICNet node. Approximately 90 percent of NCSA's off-campus users employ NSFNET. Industrial partners reach NCSA via private T1 (1.5 Mbps) circuits, and terminal servers provide dialup access.

To provide a uniform UNIX environment, Sun Network File System (NFS) and Yellow Pages are run extensively. A number of Macintosh AppleShare servers are used for document storage, collaboration, and reporting. Technologies allow files to be shared between UNIX and Mac OS so that all workstation distributed file service is accommodated with NFS. AppleTalk is currently transported over the backbone networks within IP; however, native AppleTalk routing will be part of the targeted network architecture upgrade.

Target network architecture

The networking study confirmed the need to make several changes at the high end. Although the architec-

FDDI continued on page 18

FDDI continued from page 17

ture of IP routers that separate lower speed subnets from higher speed backbones will remain, more high-end workstations will be added to the higher speed backbones. Ethernet is adequate for current-generation workstations, such as Macintosh II and Sun-3, and will remain.

A 100 Mbps Fiber Distributed Data Interface (FDDI) network will be required for many applications, particularly visualization, using Sun-4, IBM RS-6000, and high-end SGI systems. The primary backbone for workstation access to file systems and supercomputer systems will be FDDI.

A higher speed backbone will be required for supercomputer interaction, supercomputer access to high-speed file systems, and state-of-the-art visualization and distributed processing applications. This higher speed network will be based on the standard High Performance Parallel Interface (HIPPI, formerly HSC). NCSA staff members are actively involved with the ANSI committee responsible for developing the standards that are required to design a network based on the HIPPI interface.

FDDI testbed installed

Planning is underway to determine the migration schedule and strategy that is required to replace NCSA's current HYPERchannel backbone with FDDI. For example, an FDDI testbed was established as a cornerstone project in the Networking and Systems Development group. FDDI hardware selection will be made after an FDDI beta test in which extensive benchmarking and evaluation will be done in cooperation with manufacturers.

Investigation of HIPPI-class networks will continue as well, though selection of HIPPI hardware will take place over an extended period while standards specifications progress. NCSA will continue to work to provide input to a standard network architecture that will be built around the HIPPI. Cooperation with several major companies is included in this development effort.

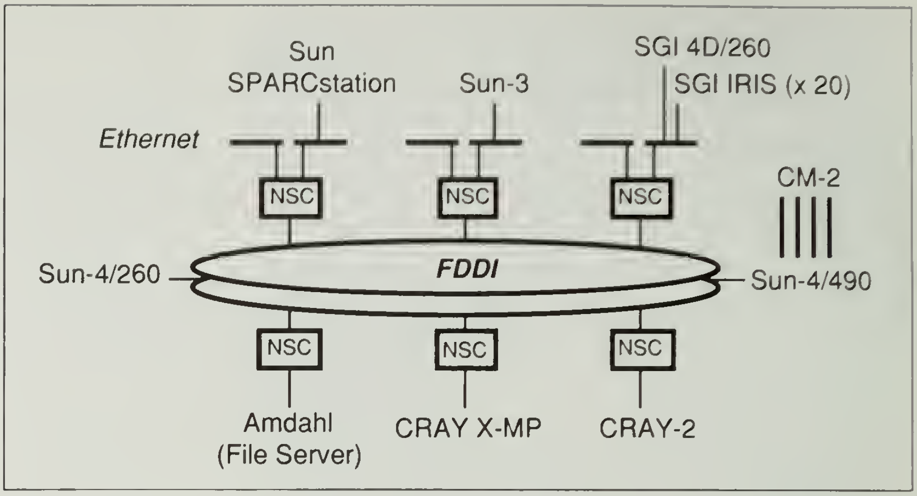


Figure 1. FDDI testbed.

In March, the NCSA FDDI testbed was installed. (See the configuration in Figure 1.) In a joint effort, a February 1990 agreement with Cray Research, Inc. and Network Systems Corporation established NCSA as a beta test site for FDDI hardware and software from these two corporations. Additional nodes from other manufacturers, including AT&T, Cisco, Sun Microsystems, Silicon Graphics, and Proteon were installed during June and July.

Testbed efforts are aimed at providing a neutral benchmarking environment. A standard set of utilities and tests are being used to evaluate performance and function of routers, bridges, and host interfaces. NCSA has developed a number of UNIX-based tools for this purpose, partially through funding from AT&T [see ***access***, February 1990].

NCSA is actively seeking additional FDDI equipment manufacturers to include in the testbed.

(See the current issue of ***data link*** for a related article entitled "Internetworking and using Internet.")

Note: This is part one of a two-part series on NCSA's networking upgrades. Major new initiatives in Gigabit per second networking research will be discussed in the September–October ***access***. ▲

Networking and Advanced Computing Workshop

by Charlie Catlett, Manager, Networking and Systems Development

NCSA will be hosting the Networking and Advanced Computing Workshop October 16 and 17 at the Beckman Institute, 405 North Mathews Street, Urbana, IL.

This gathering will combine two former annual meetings: the Networking and Supercomputing Workshop and the Parallelism and Vectorization Conference. Sandy Fraser, executive director of AT&T Bell Laboratories, will address conference participants on October 17.

The first day of this two-day workshop, the advanced computing portion of the event, will focus on massively parallel computing. It will include presentations on architectures, algorithms, and applications. The second day will involve panel discussions on networking that will include updates on WAN and LAN technology, overviews of research and development efforts including the NRI Gigabit/second network testbeds, and updates on the NSFNET backbone and international Internet.

For further information, contact Charles E. Catlett at (217) 333-1163 or catlett@ncsa.uiuc.edu (Internet) about networking aspects of the workshop; and Michael Welge at (217) 244-1999, or welge@ncsa.uiuc.edu (Internet) about advanced computing. ▲

NSF expands NSFNET

by Charlie Catlett, Manager, Networking and Systems Development

NSF recently announced a $7.9 million expansion of its nationwide computer network, NSFNET, creating the world's fastest openly available network for research and education.

In addition to adding three new nodes, or connections, to the backbone of NSFNET, data transmission speed on several key links of the existing network will increase to 45 Mbps (million bits per second).

The sites that will be linked by the higher speed connections are Cambridge, MA; Ithaca, NY; Pittsburgh, PA; Ann Arbor, MI; Urbana-Champaign, IL; Argonne, IL; San Diego, CA; and Palo Alto, CA. The technology used to support the higher transmission speeds will support the development of the proposed very high speed National Research and Education Network (NREN).

"The network is used to access resources such as supercomputers, libraries, and satellite data, as well as to link geographically dispersed researchers, educators, and scholars," said Stephen Wolff, director of the Division of Networking and Communications Research and Infrastructure at NSF.

New nodes on the NSFNET backbone network will be located at MIT, Cambridge, MA; Argonne National Laboratory, Argonne, IL; and Georgia Tech, Atlanta, GA. The Cambridge node will connect the New England Academic and Research Network (NEARnet) to NSFNET. In addition to providing connections to Argonne, the Argonne node will provide additional connections to CICnet which serves institutions in the upper Midwest. The Atlanta node will provide additional connections to the Southeastern University Research Association Network (SURAnet).

The new sites will augment the existing 13 nodes which connect midlevel networks to the network backbone. The midlevel networks in turn link computers in more than 1,000 university, government, and industrial research institutions throughout the world.

The NSFNET backbone is managed and operated by the Merit Computer Network from its state-of-the-art network operations center on the campus of the University of Michigan, Ann Arbor, MI, as part of a cooperative agreement with NSF. Merit's partners in the project include IBM Corporation, MCI Communications Corporation, and the State of Michigan through its Strategic Fund. MCI will provide advanced circuit switching technology for the expansion capable of a 28-fold increase in current backbone transmission speed. IBM will deploy a new generation of technology to take advantage of the increased capacity of the expanded network.

NCSA has operated a backbone node on NSFNET since the network was first installed in March 1986. At that time the network was a 56 Kbps (kilobits per second) network connecting six NSF-funded supercomputer centers. Today NSFNET connects over 1,600 sites including international links to Australia and the South Pacific and to Europe. The T3 upgrade this year will bring the network speed to nearly 1,000 times the speed of the original 1986 network. ▲

***Clouds** continued from page 7*

"There's also a channel in what's called the 'window' region at 12 microns that more or less gives the temperature at the top of the cloud. So you've got three measurements and maybe eight unknowns about the cloud. You try to reduce that by various physical inputs into three equations and three unknowns."

Austin's goal is to "learn enough about the clouds so that we could look at a satellite return and look at these three channels and say: 'Oh, yes, these are 12 micron drops, the cloud top is at 1 kilometer, it's 200 meters thick, and there is 30% fractional cloud cover.' If we could get that (an example of a typical cloud retrieval) from a satellite image, then we wouldn't have to fly a plane through it because we'd know how much sunlight was reaching the surface and how much the cloud was affecting the heating of the earth.

"So the idea is to let these satellites eventually stand on their own," says Austin, "and we aren't there yet." In 1992 there will be another experiment off the Azores with the same research objective focussed on broken Atlantic clouds. "It's several million dollars each time you do this," Austin notes. He explains further that these clouds are in a different climatic regime. There will be measurements from an oceanographic experiment that will be conducted simultaneously. Much of what was learned in 1987 will be applied to the 1992 study. "The hope is that if you do this twice, you'll have enough data [that] you can start developing some physical models for these clouds."

Imaging with NCSA tools

"Organizing the aircraft data is quite a chore because there are about 3,400 channels being measured every second," says Austin. "So it was a major gift for us to find NCSA-produced software ready made."

NCSA X Window software tools (NCSA X Image and NCSA X DataSlice) together with HDF (Hierarchical Data Format) for data organization and transport between systems is used considerably in Austin's work.

"A year ago, our satellite lab had a single VAX 11-750, one color terminal, and image-processing software developed in-house." New research funding recently brought money for 10 new workstations. "X Image allowed us to get images from various sources, put them in HDF format, and look at them on our workstations instead of waiting in line at one terminal for this VAX," Austin continues.

"The nicest thing about HDF has been the ability to store and document binary data. X DataSlice has spread to the atmospheric modelers in our group. They have been using it in visualization of 3D gridded numerical model output. They had some nice view graphs for the Canadian Meteorological and Oceanographic Society Conference in Victoria, and we credit NCSA for that." ▲

***Air pollution** continued from page 5*

Educating the public

Although the video has been accepted for showing at SIGGRAPH '90, McRae regards it as a "first draft" of an ongoing project. Agencies to whom he has shown the visualization are interested in funding a longer version, he says, that can be released to television stations on days of high pollution to show people what is happening in the air. The visualization could also be used as an educational tool to explain air pollution and what can be done to improve air quality.

The federal Clean Air Act amendments now in Congress provide for state and local governments to implement air quality improvements. This act will likely increase demand for presentations like this video. According to McRae, California is important to research on air pollution because it leads the country in air quality planning, and LA sets the pace for the rest of the U.S. "What you'll see is that this [video] will become a lot more impressive," he says. "It will be used as part of an educational campaign." ▲

Thanks for your response

Your response to the "Newsletter Survey" that we mailed to you with the April newsletters was overwhelming. In fact, so many readers responded that we were still tabulating and analyzing the results a week after the deadline.

We estimate that more than 11%, or 670, of you took the time to answer our questions and write down some comments about ***access*** and ***data link***. According to the experts, that is about twice the usual reply to expect.

Your input is invaluable. Thanks. In the next issue of ***access***, we will report on your survey response.

*—Fran Bond, Editor of **access***

***Refining ozone** continued from page 3*

These are the primary ozone depletion cycles. Each cycle results in the destruction of ozone by converting it to O_2. But more importantly, each cycle operates catalytically—that is, each cycle concludes by again freeing the destructive radical to attack more ozone. For example, each chlorine molecule can destroy as many as 100,000 ozone molecules before it becomes inactivated by combining with a substance outside of the depletion cycle. (Chlorine is the free radical born of the breakdown of CFCs.)

Searching for a solution

Turner and his colleagues have embarked on a slow, painstaking process of discovery. They are searching for equations that link the primary cycles so that their depletion models will better resemble true atmospheric chemistry. Their goal is to build more complete models that match reality. Says Turner, "By finding the coupling equations we hope to refine the depletion model and make it more useful to the scientific community."

Specifically, Turner and his associates use state-of-the-art quantum mechanical methods performed on NCSA's Cray system to examine the stability of various molecules and the *topology,* or map, of the associated potential energy surfaces. With this information, Turner can calculate rate constants for proposed coupling reactions. The rate constant tells him how rapidly a reaction occurs with respect to other reactions in the cycle. If the rate is low, the reaction probably doesn't occur with enough frequency to influence the depletion cycle. If it is high, the reaction is likely to happen, and it becomes a candidate for study.

"We're using iterative computational techniques to study the chemical cycles of ozone depletion," says Turner. "You can't begin to do this without a supercomputer. The methods that we use lead to CPU-intensive calculations. The calculations also require large computer memory."

Solving the equations enables the scientist to predict with certainty how the molecule will behave in the presence of other substances. Each of Turner's solutions is a small piece in the ozone depletion puzzle—a difficult but important step forward. Turner conducts his research at NCSA remotely via NSFNET and uses GAUSSIAN88, a standard quantum chemistry package. "This year we'll be working on the CRAY-2," he says. "Its large memory will enable us to expand our work and to get faster results."

Turner and his research team have clues as to where couplings may occur. For example, molecules such as nitrosyl chloride (NOCl) and its valence isomer chloride nitrosyl (ClNO), may serve as "sinks" for the removal of active species in the cycles, or may themselves undergo reactions which modify the depletion of ozone. According to Turner, sinks tie up chlorine and reduce ozone. "From studying energetics we know NOCl is a sink," says Turner. "But we must also study the photodissociation cross sections in order to know the whole picture."

The *photodissociation cross section* examines the stability of a compound under bombardment by stratospheric sunlight. At ground level, NOCl would tend to tie up both free radicals—NO and Cl—making them unavailable for ozone depletion. But the high-energy sunlight of the stratosphere may be able to break this molecule apart and free the radicals again for ozone destruction. Turner's goal is to determine whether this breaking, or *photolysis*, is occurring.

So far Turner's study has focused entirely on primary-primary coupling reactions—that is, reactions between Cl, NO, and OH. The next step will be to examine primary-secondary reactions, namely reactions between the primary radicals (Cl, NO, OH) and other species which occur in the depletion cycles, for example $Cl + NO_2 = ClNO_2$ or $OH + ClO = HOClO$, etc. Later Turner hopes to expand to secondary-secondary reactions, including reactions in condensed phases. (Condensed phases include water or ice crystals in stratospheric clouds.)

Environmentalists concur that reducing the emission of pollutants is a step toward solving problems. Yet they also agree that the effects of any environmental change probably cannot be measured for a decade.

For now, Turner and his colleagues will continue their search. "Pollutants play a major role in ozone depletion, and *at present* there are no practical solutions to this problem," says Turner. "Our ultimate goal of course is to reveal solutions. This is a very serious problem that threatens us all." ▲

New and updated online information

by Will Ridenour, Online Documentation Editor

The following help files, documents, and man pages have been added or updated as of July 3, 1990.

UNICOS help files

Name	Description
access campus-connections	Information about local access to NCSA
calendar holiday	Scheduled UIUC holidays
calendar training	Scheduled NCSA user training
training	Information about NCSA user training
unicos nqs	Information about the network queuing system

ULTRIX help files

Name	Description
access campus-connections	Information about local access to NCSA
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unicos nqs	Information about the network queuing system

To access a help topic on either Cray system or ncsagate, enter: **`help topic`**
where *topic* is the name of the topic you wish to view.

UNICOS man pages

Name	Description
acm-algorithms	Collection of math subroutines
areas	Creates an area map from a set of edges
autograph	Draws curves or families of curves
cazm	Circuit analyzer with macromodeling
cftmath	General purpose math library
cgm2ncar	Filter NCAR CGM to/from vanilla CGM
cgm-edit	X window interface to the NCAR View cgm library
cgmtrans	NCAR CGM translator
colconv	Converts color values from one color space to another
conpack	Contours regularly distributed (gridded) data
conran	Contours irregularly spaced data, labeling lines
conraq	Contours data, no labeling
conras	Contours data, lines smoothed, crowded lines removed
conrec	Contours 2D arrays, labeling contour lines
conrecqck	Contours 2D arrays, no labeling
conrecspr	Contours 2D arrays, lines smoothed, crowded lines removed
ctrans	CGM translator
dashchar	Software dashed-line package with character capability
dashline	Software dashed-line package
dashsmth	Software dashed-line package with character capability and smoothing
dashsupr	Software dashed-line package with character capability, smoothing, and the capability of removing crowded lines
ecmfft	Fast Fourier transform package
ezmap	Plots world/regional border outlines
ezmapa	Allows EZMAP output redirection to AREAS routines
findg	Locates calls to all entries in pre-GKS NCAR Graphics
fontc	Fontcap preprocessor for NCAR Graphics
fontcap	NCAR Graphics font definition file
ftrans	NCAR CGM translator
gflash	Captures and inserts specified portions of graphics instructions in subsequent frames
graphc	Graphcap preprocessor for NCAR Graphics
graphcap	NCAR Graphics graphic device definition file
gridal	Draws background grids
hafton	Halftone pictures of 2D arrays
histgr	Plots histograms
hspice	Circuit simulation program
idt	X window interactive interface to NCAR View image displaying tools
isosrf	Iso-surfaces from 2D arrays, hidden lines removed
isosrfhr	Iso-surfaces from high-resolution 3D arrays
kap	Vectorizing/concurrentizing FORTRAN preprocessor
labelbar	Creates a labeled, filled, rectangular bar to serve as a key for a filled plot
mc	Checks monotonicity of CAzM tables
ncar2cgm	Filter NCAR CGM to/from vanilla CGM
ncargcc	Command for compiling C code that uses NCAR Graphics

***Online information** continued on page 22*

***Online information** continued from page 21*

ncargrun	Front-end script for NCAR GKS utilities
ncargtest	Creates, compiles, links, a program that uses an NCAR Graphics utility
pisces	2-carrier, 2D semiconductor device modeling program
plotchar	Plots text using one of three quality levels
plt	User interface for NCAR metacode translators
pwritx	Fancy character plotting
pwrity	Character plotting
pwrzi	Plots characters in 3D with ISOSRF
pwrzs	Plots characters in 3D with SRFACE
pwrzt	Plots characters in 3D with THREED
scilib	Math library from Cray Research, Inc.
softfill	Fills the area inside a polygon in various ways
spice	Circuit simulation programs
spice2g5	Circuit simulation program version 2g5
spice2g6	Circuit simulation program version 2g6
spice3b1	Circuit simulation program version 3b1
srface	3D plot of functions with 2 variables
stitle	Plot stationary or scrolling titles
strmln	Draws a streamline representation of a flow field
suprem	Process modeling program for semiconductor devices
table	Changes CAzM tables between ASCII and binary formats
umspice	Circuit simulation program
velvct	Draws 2D velocity fields

To access a UNICOS man page enter: `man manpage` where *manpage* is the name of the man page you wish to view.

UNICOS documents

Name	**Description**
dassl.doc	Describes the dassl mathematics library
cfs	Describes the common file (mass store) system

To access dassl.doc or other documents in /usr/local/doc, change directories to /usr/local/doc and enter: `more docname` where *docname* is the name of the document you wish to view.

To access cfs or other documents in docview, enter: `docview view docname` where *docname* is the name of the document you wish to view. ▲

Tentative training dates: 1990*

August 20–24	Cray Code Development Training
September 17–19	Cray Applications** Training
October 8–12	CM-2 Training
October 17–18	Networking/Advanced Computing Workshop
October 22–26	Affiliates Training
October (TBA)	Visualization Workshop
November 5–9	Cray Code Development Training
December 3–5	Cray Applications** Training

You must register to attend NCSA Training. Class size is limited.

To register Academic users contact Karen Gobble at (217) 244-4198. Industrial partner users contact your representative at NCSA. Academic affiliates contact Kendra Reasor at (217) 244-1100.

For additional information Contact Lyle Rigdon at (217) 244-3659 or lrigdon@ncsa.uiuc.edu (Internet) or 26818@ncsavms (BITNET).

***PLEASE NOTE** These dates are subject to change.

**Applications will be in the fields of chemistry, finite element, and computational fluid dynamics.

NCSA contacts

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bottum@ncsa.uiuc.edu (Internet)

Anonymous FTP IP address
ftp.ncsa.uiuc.edu (128.174.20.50)

CM Sun front-end address
cmsun.ncsa.uiuc.edu (128.174.220.4)

CM VAX front-end
cmvax.ncsa.uiuc.edu (128.174.220.5)

Cray operations
(217) 244-0710

CRAY X-MP IP address
ux.ncsa.uiuc.edu (128.174.10.46)

CRAY-2 IP address
u2.ncsa.uiuc.edu (128.174.10.44)

Dialup access—2400 baud or less
(217) 244-0662

Dialup access—9600 baud
(217) 244-6733

NSF Network Service Center
nnsc@nnsc.nsf.net

NSFNET problems
(617) 873-3400

SRI-Network Information Center
(415) 859-3695
nic.ddn.mil

VAX/ULTRIX gateway addresses
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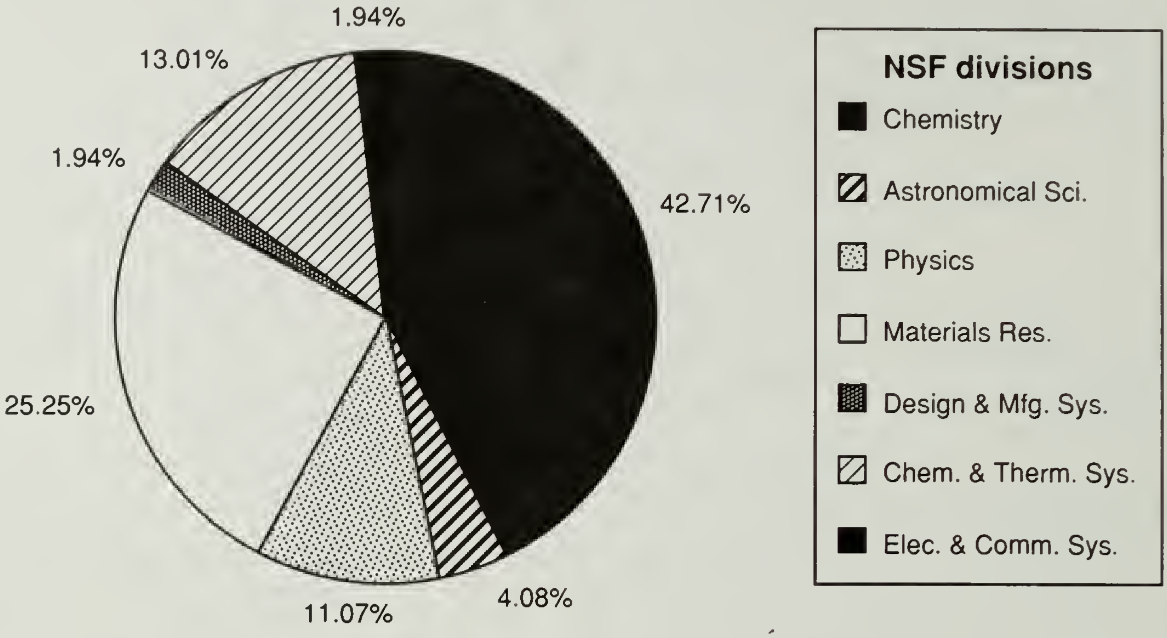
14998@ncsavms (BITNET)
dbrady@ncsa.uiuc.edu (Internet)

June '90 PRB service units allocated (by area of science/engineering)



Total number of services units allocated were 5,149. For further details about the most recent allocations made by the Peer Review Board, see the accompanying flier.

data link contents

- Hot tips and topics
- Print to local UNIX printers with lpr
- NQS turnaround statistics now available
- Changes to NQS on the CRAY X-MP system
- Internetworking and using Internet
- RPAC available on the NCSA Cray systems
- CAzM circuit simulator now available
- NCAR Graphic updated to 3.0

To receive a copy of the current issue of ***data link***, contact the NCSA receptionist at (217) 244-0072.

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Mail to Tammie Hildreth, Information and Publications, NCSA ***access***,
152 Computing Applications Building, 605 E. Springfield Ave., Champaign, IL 61820.

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the NCSA newsletter
November–December 1990 vol. 4 no. 8

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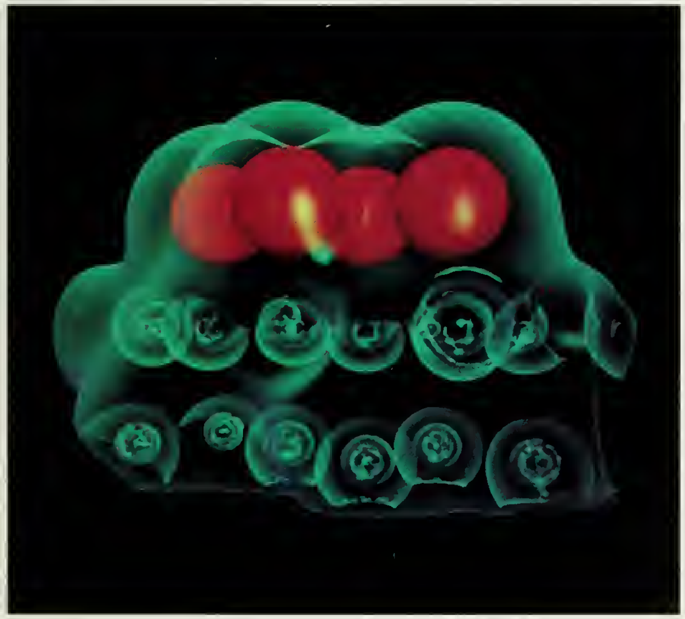
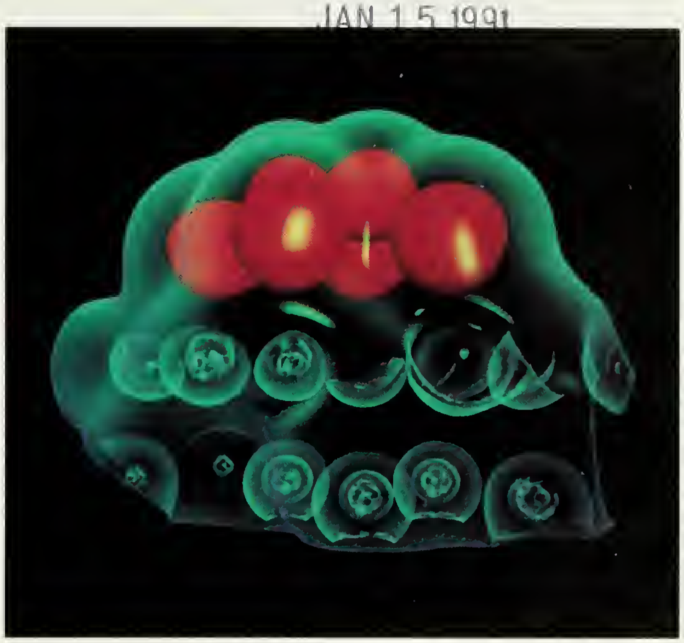
Computational chemistry at NCSA

"It is the great beauty of our science, CHEMISTRY, that advancement in it, whether in a degree great or small, instead of exhausting the subjects of research, opens the doors to further and more abundant knowledge, overflowing with beauty and utility, to those who will be at the easy personal pains of undertaking its experimental investigation."—Michael Faraday (1791–1867) from *Experimental Researches in Electricity* as quoted in *Great Treasury of Western Thought* (Mortimer S. Adler and Charles Van Doren, editors).





Chemisorption and dissociation of a nitrogen molecule on a palladium surface. These images show the 20-atom cluster model of the surface of palladium before (left) and after (right) a nitrogen molecule binds. Surfaces are of constant electron density. The red surface, having the value of 0.1 electron per cubic bohr, contains 90% of the electron density in the chemisorption, or active, site. The green surface has the value of 0.005 electron per cubic bohr and indicates the spatial extent of the system. The bubble-like structure present in the lower layers is caused by the nodal structure of the metal atom valence orbitals. Electron densities were computed on the CRAY-2 and IBM RS/6000 systems at NCSA. [See text, page 4.] (Credits: Harrell Sellers, research; Mike Krogh, visualization; DISCO and Wavefront, software—pages 1 and 3.)

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NOTE: Italicized titles indicate sidebars or boxed information. Boxes may not follow the topics of the heads under which they fall.

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Abbreviations

ACM	Association of Computing Machinery
CRI	Cray Research, Inc.
NCSA	National Center for Supercomputing Applications
NSF	National Science Foundation
UIC	University of Illinois at Chicago
UIUC	University of Illinois at Urbana-Champaign

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High-Performance Computing Events 1991 Edition January–June

January

***January Small Allocation Committee Meeting**
Proposal deadline: December 3, 1990

***New User Training—Cray Applications**
NCSA at UIUC
January 14–16, 1991

Seventh Annual Computer Graphics Show
New York, NY
January 15–17, 1991
(301) 587-4545—David Small

Winter 1991 USENIX Technical Conference
Dallas, TX
January 21–25, 1991

PADS, Workshop on Parallel and Distributed Simulation
Anaheim, CA
January 21–23, 1991
(804) 221-3458—David M. Nicol

Second ACM–SIAM Symposium on Discrete Algorithms
San Francisco, CA
January 28–30, 1991
(215) 386-7999

April

***April Small Allocation Committee Meeting**
Proposal deadline: March 1, 1991

Dasfaa 91, Second International Symposium on Database Systems for Advanced Applications
Tokyo, Japan
April 2–4, 1991
81 (92) 641-1101, ext. 5407—
Yahiko Kambayashi

1991 Symposium on Applied Computing
Kansas City, MO
April 3–5, 1991
Deadline: November 1990

Computer Graphics and Education 91
Barcelona, Spain
April 4–6, 1991
Abstract deadline: November 1990
(209) 667-3176—Steve Cunningham

IEEE Infocom 91, Conference on Computer Comm.
Miami, FL
April 7–11, 1991
(415) 859-5710—N. Shacham

May

***May Small Allocation Committee Meeting**
Proposal deadline: April 1, 1991

22nd Annual Pittsburgh Conference on Modeling and Engineering
Pittsburgh, PA
May 2–3, 1991
Unpublished papers deadline:
January 31, 1991

***New User Training—Cray Code Development**
NCSA at UIUC
May 13–17, 1991

ICSE 13, 13th International Conference on Software Engineering
Austin, TX
May 13–17, 1991
(512) 338-3330—Bryan Fugate

CompEuro 91, IEEE International Conference on Advanced Computer Technology Reliable Systems and

both experimental and theoretical chemists. Armed with advanced spectrometers and scanning tunneling electron microscopes, experimental chemists are *now* able to see atoms and understand their behavior in many situations.

But catalysis seems to be mostly reserved for theorists like Sellers. It is difficult to study experimentally because it involves reagent atoms that are weakly bonded to a cata-

Typically, he studies a specific catalyzed reaction. For instance, a current project focuses on the bonding of acetylene to palladium. First, he solves the Schrödinger equation for all molecules involved in the reaction, including the catalyst. This tells him how the molecules ought to behave

Computational catalysis *continued on page 4*

High-Performance Computing Events 1991 Edition
January—June

January

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(804) 221-3458—David M. Nicol

Second ACM–SIAM Symposium on Discrete Algorithms
San Francisco, CA
January 28–30, 1991
(215) 386-7999

February

***February Small Allocation Committee Meeting**
Proposal deadline: January 2, 1991

Supercomputing Europe '91
Stuttgart, Germany
February 6–8, 1991
Annemarie J.W. Tiebout-de Jong
P.O. Box 8500
3503 RM Utrecht
The Netherlands

Fifth International Conference on Modeling Techniques and Tools for Computer Performance Evaluation
Torino, Italy
February 13–15, 1991
39 (382) 391-350—
Maria Carla Calzarossa

***New User Training—Cray Code Development**
NCSA at UIUC
February 18–22, 1991

March

***March NCSA/PSC Peer Review Board**
Proposal deadline: February 1, 1991

***March Small Allocation Committee Meeting**
Proposal deadline: February 1, 1991

***New User Training—Connection Machine**
NCSA at UIUC
March 18–22, 1991

1991 AEC EXPO West
San Francisco, CA
March 19–21, 1991
Deadline: December 1990
(800) 766-EXPO

National Net'91
Washington, DC
March 20–22, 1991
(202) 872-4200—
Elizabeth C. Barnhart

Symposium on Experiences with Distributed and Multiprocessor Systems
Atlanta, GA
March 21–22, 1991
Paper deadline: November 1990
(813) 530-2376—George Leach

Fifth SIAM Conference on Parallel Processing for Scientific Computing
Houston, TX
March 25–27, 1991
Deadline: October 1990

April

***April Small Allocation Committee Meeting**
Proposal deadline: March 1, 1991

Dasfaa 91, Second International Symposium on Database Systems for Advanced Applications
Tokyo, Japan
April 2–4, 1991
81 (92) 641-1101, ext. 5407—
Yahiko Kambayashi

1991 Symposium on Applied Computing
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(209) 667-3176—Steve Cunningham

IEEE Infocom 91, Conference on Computer Comm.
Miami, FL
April 7–11, 1991
(415) 859-5710—N. Shacham

IMS 91, First IEEE International Workshop on Interoperability in Multidatabase Systems
Kyoto, Japan
April 8–9, 1991
(317) 494-1998—
Ahmed K. Elmagarmid

ASPLOS 4, Fourth International Conference on Architectural Support for Programming Languages and Operating Systems
Santa Clara, CA
April 8–11, 1991
e-mail rau@hplabs.hp.com—Bob Rau

Seventh International Conference on Data Engineering
Kobe, Japan
April 8–12, 1991
(614) 292-1837—Ming T. (Mike) Liu

Supercomputing Japan 91
Tokyo, Japan
April 10–12, 1991

***New User Training—Cray Applications**
NCSA at UIUC
April 15–17, 1991

Fourth International PHOENICS User Conference
Miami Beach, FL
April 15–19, 1991
(205) 830-2620—CHAM of America

SUPER!
University of Utah
April 21–24, 1991
(801) 581-5253—Julio Facelli,
DeeAnn Raynor

NCGA 91, 1991 National Computer Graphics Association Conference
Chicago, IL
April 22–25, 1991
(703) 698-9600

IBM Large-Scale Computer Analysis and Modeling Conference
Park City, UT
April 24–26, 1991
Paper deadline: January 15, 1991
(203) 794-1355—
IBM Competition Admin

CHI 91, 1991 Conference on Human Factors in Computing Systems
New Orleans, LA
April 27–May 2, 1991
(206) 865-3389—Keith Butler

***Affiliates Training**
NCSA at UIUC
April 29–May 3, 1991

May

***May Small Allocation Committee Meeting**
Proposal deadline: April 1, 1991

22nd Annual Pittsburgh Conference on Modeling and Engineering
Pittsburgh, PA
May 2–3, 1991
Unpublished papers deadline:
January 31, 1991

***New User Training—Cray Code Development**
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May 13–17, 1991
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CompEuro 91, IEEE International Conference on Advanced Computer Technology Reliable Systems and Applications
Bologna, Italy
May 13–17, 1991

International Symposium on Software Reliability Engineering
Austin, TX
May 17–18, 1991
(904) 474-2989—John Munson

ICDCS 91, 11th International Conference on Distributed Computing Systems
Arlington, TX
May 20–24, 1991
(817) 273-3785—Bill D. Carroll

Second International Conference on Algebraic Methodology and Software Technology
Iowa City, IA
May 22–24, 1991
Abstract deadline: January 1, 1991

World Computer Law Conference
Chicago, IL
May 23–25, 1991
(213) 689-5186—Michael D. Scott

ICCI 91, International Conference on Computing and Information
Ottawa, Canada
May 27–29, 1991
Paper deadline: November 1990

Fifth Israel Conference on Computers Systems and Software Engineering
Herzlia, Israel
May 28–29, 1991
Abstract deadline: December 14, 1990
972 (3) 664-825—M. Winokur, TelAviv

June

***June NCSA/PSC Peer Review Board**
Proposal deadline: May 1, 1991

***June Small Allocation Committee Meeting**
Proposal deadline: May 1, 1991

CVPR 91, IEEE Computer Society Conference on Computer Vision and Pattern Recognition
Lahaina, Maui, HA
June 3–7, 1991
Paper deadline: November 1990
e-mail shahriar@wiliki.eng.hawaii.edu

Symposium on Solid Modeling Foundations and CAD/CAM Applications
Austin, TX
June 5–7, 1991
Abstract deadline: October 1990
(914) 784-7455—Jaroslaw Rossignac

SCM3, Third International Workshop on Software Configuration Management
Trondheim, Norway
June 12–14, 1991
Paper deadline: November 1990
(412) 268-7790—Peter Feiler

***New User Training—Cray Applications**
NCSA at UIUC
June 17–19, 1991

Eighth International Conference on Testing Computers Software
Washington DC
June 17–21, 1991
Abstract deadline: November 1990
(301) 266-8244—
Genevieve Houston–Ludlam

Supercomputing USA/Pacific 91
Santa Clara, CA
June 19–21, 1991

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Enter `help calendar high-performance` to access an online version of this calendar on the Cray systems.

National Center for Supercomputing Applications
University of Illinois at Urbana-Champaign

Computational catalysis

by Randall Graham, Science Writer

If atoms were as big as golfballs, it might be easy to understand how a catalyst accelerates chemical reactions. We could watch chemical bonds being broken and reconstructed and see how the atoms of the catalyst influence the process. But atoms are so small and move so fast that actually seeing how they interact is all but impossible.

There is another way to study molecules, however. The secrets of their behavior are locked within Newton's laws and the Schrödinger equation. Yet only in the last few years have supercomputers been developed that can handle the computations. Harrell Sellers, NCSA senior research scientist in surface chemistry, is using the CRAY-2 system to solve the fundamental equations for reactions of surface catalysts.

"The supercomputer is our best microscope for this sort of study," says Sellers. "With it we're able to see exactly where atoms are and what they're doing." Sellers solves equations and simulates molecular interactions.

Catalytic activity is an essential industrial chemical process. It virtually drives the multibillion-dollar petroleum, chemical, and pharmaceutical industries and accounts for a large percentage of all goods produced in the U.S. Discovering how catalysis works would be like unearthing a gold mine, because scientists could then develop new catalysts and refine existing ones without having to guess at the results.

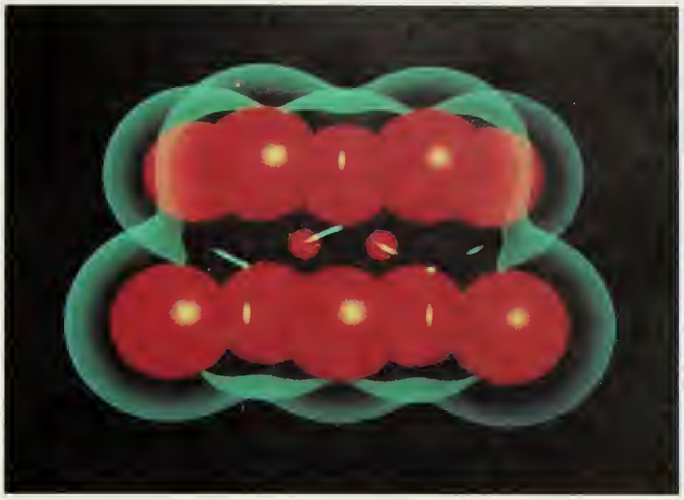
Seller's work is part of a Grand Challenge effort. "Our Grand Challenges in this field are" says Sellers, "to uncover the rules that govern catalysis—those laws that explain how it works. It won't be easy and may not even be accomplished in my lifetime, but finally we have the methods and computing power to begin."

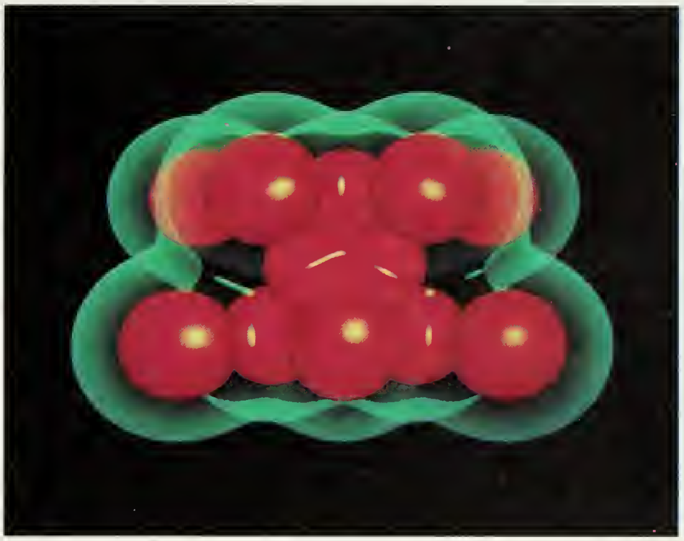
Sellers is developing the methods. NCSA has the computing power. "NCSA is one of the finest computing facilities in the world. It has all the tools I need, tremendous hardware, and high-quality people. I can go down the hall and talk to somebody in Cray operations about a problem I'm having with a program and get it solved. It also has a thriving industrial program, so I get to work with many companies on their specific projects. While assisting them, I also advance the field of computational catalysis."

Theory and experiment

Other areas of chemistry are yielding their secrets to both experimental and theoretical chemists. Armed with advanced spectrometers and scanning tunneling electron microscopes, experimental chemists are *now* able to see atoms and understand their behavior in many situations.

But catalysis seems to be mostly reserved for theorists like Sellers. It is difficult to study experimentally because it involves reagent atoms that are weakly bonded to a catalytic surface. This presents two problems. Surface atoms have always been more difficult to look at than atoms in the gas or liquid phase, and molecules bonded weakly to those surfaces, as they are during catalysis, are easily disrupted or scraped off by scanning technologies. "The best way to gain an understanding of catalysis on a microscopic level is with computational methods," observes Sellers.





Interstitial (interior) chemistry. Images of a hydrogen molecule (above) and an oxygen molecule (below) in the cavity of a simulated palladium crystal. [See text, page 4.]

Sellers employs ab initio methods. *Ab initio* means "from the beginning" in Latin, and it refers to any method based solely on fundamental physical principles rather than equations with an experimental root. Sellers solves problems using either Newton's laws of motion or the Schrödinger equation, the fundamental equation for determining quantum molecular properties.

Typically, he studies a specific catalyzed reaction. For instance, a current project focuses on the bonding of acetylene to palladium. First, he solves the Schrödinger equation for all molecules involved in the reaction, including the catalyst. This tells him how the molecules ought to behave

Computational catalysis *continued on page 4*

Computational catalysis continued from page 3

during the reaction based on their shape, physical properties, and available bonding sites. This step may require many hours on a high-performance computer.

Next Sellers makes predictions about the reaction: what sites the reagents will bond to, why they will bond there, and what the various resulting products will be and in what proportion. Finally he evaluates his predictions by comparing them with experimental results. If no experimental results are available, and this is often the case, he tries to get someone to generate them. "Basically I try to talk someone into doing the experiment I need. We desperately need those results to tell us how well we're doing in our modeling effort."

Since the computations are so lengthy, Sellers attempts to simplify them by using as few as ten to twenty metal atoms to represent an infinite surface. "It was once thought you would need hundreds of atoms to represent a surface," says Sellers. "But techniques have now been developed that allow us to mimic an infinite surface with very few atoms by manipulating the electronic structure of the system. This greatly simplifies the calculations."

Rewarded effort

Discovering the laws of catalysis is still a distant dream, but work toward it is already bearing fruit. Sellers and his colleagues are learning how to design new catalysts and improve old ones using computer hours instead of man-years to accomplish the task. "Given enough computer time, there are many games we can play to enhance the specificity of a catalyst. For instance, different faces of a crystal have different chemical properties. We can look at how the same chemicals behave in the presence of these different surfaces. We can also study the catalytic properties of systems with more than one metal or metals on, say, a graphite substrate—or even surfaces with holes in them where atoms are missing."

Part of the attraction NCSA holds for its industrial partners is the potential to save money by simulating costly experiments on the supercomputer. "In one project with Eli Lilly, we were trying to understand the mechanics of a certain catalyzed hydrogenation reaction. We hypothesized that two different reaction mechanisms were occurring. To find out if this was reasonable, I did some ab initio calculations to see if both pathways were energetically feasible. They were. Now the next step may be to go to the lab and try to block the undesirable mechanism. The point is, we were able to make significant progress on this problem outside the lab, using the supercomputer."

Engineered coatings

A field related to catalysis that fascinates Sellers is that of engineered coatings. *Engineered coatings* are a means of endowing objects with desirable properties by dipping them in solutions that chemically bond to their surface. The process resembles painting, but the technology is quite different. "These engineered coatings are pseudocrystalline in nature. That means they bond to objects in an ordered monolayer, an ultrathin layer in which all the molecules are lined up the same way."

While some bonding may occur with paints, engineered coatings bond to an object completely. A coat of paint is thousands of molecules thick, but an engineered coating may be only one, two, or three molecules deep. Such ultrathin coatings may some day have many applications—preventing the human body from rejecting surgical implants, developing very high resolution photographic film, or applying permanent lubrication or corrosion resistance to objects. "I compare engineered coatings to high-temperature superconductors as far as their significance to the scientific community is concerned. At present there are very few actual applications for either technology, but everyone is excited by the potential of high-temp superconductors. Engineered coatings have that same kind of potential. I'm excited because their pseudocrystalline nature also makes them easier to model on the supercomputer."

Method development

Writing computer codes is another part of Seller's work. Streamlining calculations to save computer time is essential to advancing his work. Sellers uses the DISCO code, public domain software originally developed in Jan Almlöf's group at the University of Oslo in Norway (see page 7). "I've tailored my version so much to my own needs that parts of it differ very significantly from the original program. One of the differences that I have installed in DISCO is the ability to treat individual metal atoms as sources of electrostatic potential only. The result is [that] the size of the calculation does not increase just because we add 'bulk' metal atoms to the model. It's one way to simplify the calculations."

Harrell Sellers. (Photo by John Melchi, Public Information Intern.)

Graphics effort

Sellers is also spearheading an aggressive graphics research effort using the CRAY-2 system and an IBM grant that provides him with IBM's powerful RS/6000 computer. "We utilize the Cray-2 and the IBM RS/6000-530 machine in our surface chemistry and catalysis modeling. I found that the IBM RS/6000 runs the vectorized code DISCO at a CPU speed of one-fourth that on a single-processor CRAY-2, thereby giving wall-clock turnaround comparable with the Cray run in single-processor mode. It is a very powerful machine and a very valuable resource; we keep it fully loaded at all times. Our strategy in this computing environment is to keep our largest calculations on the Cray-2 and keep

***Computational catalysis** continued on page 14*

Keeper of the codes

by William Dwyer, Graduate Assistant Writer

"People use codes like they eat ice cream," explains Joe Golab, new head of NCSA's Computational Chemistry Group. Golab points to binders of documentation that fill the shelves in his Beckman Institute office. He says that users rarely want to try new, perhaps better, codes if it means giving up the ones with which they are already familiar. "If they grew up eating vanilla, they're not going to start eating chocolate, unless they have a reason—a good reason."

Golab hopes to provide users with such "good reasons" for using the latest software. He has written experimental interfaces that take care of many of the "nonchemistry" requirements for running chemistry applications software, and he is working on a more sophisticated interface that will accept a user's data in most formats and then select the most efficient program to run that job.

Golab's objective is to make the codes more than just "user friendly." "Some people like 'user amorous,' but that sounds too lovey-dovey," he explained. "The way I see myself is to make these codes 'user affectionate.'" According to Golab, the codes should be "easy to run, reliable, and effective."

Untangling codes

At NCSA's new user training sessions, Golab tells participants that they should not think of a chemistry code as a "magic black box." They cannot expect programs to understand what to do with their data. If a code cannot interpret the data, the situation amounts to putting in junk and getting junk back, he says. And even if the machine gives back the right numbers, it does not interpret them for the user.

Another problem Golab explains to new users is that most codes used for chemistry research originated in an academic environment, where programmers do not concentrate on documentation or making the codes tolerant to abuse. For that reason, Golab says the codes could have been written in Sanskrit as far as the average researcher is concerned.

Golab's solution has been to write so-called Qscripts, which interface with individual programs and the NQS queueing system on the Cray systems.

After logging on, Cray users at NCSA can eliminate many of the nonchemistry program requirements by running a Qscript for that code. Qscripts determine queueing system parameters, such as memory size, what queue to use, and the time-block required for running a job. Other supercomputing centers have their own versions of Qscript, Golab says, but each script is designed for particular software and user requirements.

"It was an experiment that worked," says Golab, who has written experimental Qscripts for GAUSSIAN88, GAMESS, and RPAC—three codes that represent a range of problems the interface encounters. (GAUSSIAN88 and GAMESS, along with MOPAC and CHARMm, are the most frequently used chemistry codes at NCSA.) Writing Qscripts for the remaining codes will be "a matter of replication." Golab now has a graduate research assistant, Mark Foy, to assist in writing the Qscripts and to compare code characteristics for their most useful and efficient application. Foy, who has experience in artificial intelligence, will also work to make the Qscripts more helpful and intuitive for users.

"Joe has been doing a very good job making user codes as friendly as they are," says Harrell Sellers, NCSA senior research scientist in surface chemistry and former head of the Computational Chemistry Group. "He enjoys talking to users—he's very good at it—and users find him easy to talk to," adds Sellers, who is now in charge of the Computational Catalysis team in the Materials Science Group (see page 3).

Golab says he will know that he has succeeded in his quest to satisfy user needs when he no longer has people calling or sending him electronic mail. If that happens, he would no longer be needed. But it won't happen—at least for a while yet, because he plans to continue making improvements to the interfaces.

Joe Golab. (Photo by John Melchi, Public Information Intern.)

Helping NCSA's users

Research will play a significant role in Golab's attempts to help academic and industrial users solve their unique problems. Golab gives as an example a chemistry professor he helped with calculations of parameters for estrogen-related compounds. The parameters were used in a public domain program called CHARMM, which the professor had modified for his particular needs. The result, Golab says, were some interesting and unexpected quantifiable conclusions.

Golab mentions that his research tries to define "comprehensive computational approaches to chemical questions." And he continues to maintain and update documentation for chemistry codes, the software programs used on the supercomputers. He says he will continue to provide users with instructions for running the codes, so that chemists' time can be better spent, as he says, "doing chemistry."

"I've really appreciated what [Golab] has done in terms of helping me get on the Cray—getting me up and running," says Andy Holder, an academic user from the University of Missouri at Kansas City, who does very large calculations on the supercomputers at NCSA. Holder uses GAUSSIAN88 for ab initio calculations on, for example, homotropylium cations. He is working to determine the geometry and properties of the cations' seven-member carbon ring structure.

Codes *continued on page 6*

Codes continued from page 5

Holder says his association with Golab has been one of mutual exchange. He provided Golab with the latest version of a code called AMPAC and one called AMPGAUSS.

Continuing improvements

Golab used AMPGAUSS to develop a prototype translator, which will take a user's input and—no matter which program's input format it is in—translate and run that input with the most efficient code for solving the chemistry problem. When the translator is ready, it will also serve Golab's goal to free users from having to think about what programs to run so they will have more time to do chemistry. And the translator will eventually be linked with Qscripts so users won't even have to decide whether they need to use the translator. The Qscripts will do it for them.

"The idea is to keep making this interface (between users and codes) better and better," says Golab. He already has a prototype translator working now, and David Deerfield, biomedical scientific specialist at the Pittsburgh Supercomputing Center (PSC), is collaborating with him to improve the design.

"One of my hopes would be to put some intelligence in the programs to make sure they are used most efficiently," Deerfield says, noting that user needs are similar at both NSF-sponsored centers. "The translator would provide users with more intelligence on which software would be best" for their needs.

Partnering in research

Referring to Golab's translator project, "I'm excited about the things he's thinking about," says Jim Rieke, onsite representative of NCSA industrial partner Dow Chemical Co. Rieke says Golab's work puts software applications into the hands of chemists, who "don't have to be specialists" in computational science.

"Joe's been helpful in many ways getting our people started," says Rieke.

In his office at NCSA, Rieke sketches a "science stool," which has two sturdy "legs": theory and experiment. A third spindly leg represents computational science. He explains that the tools are now available to make the computational science leg as strong as the other two.

Rieke acknowledges Golab's contribution to the effort: "Joe will provide a valuable service by making quantum chemistry available to scientists at a level that is appropriate for the task to be done."

"Ultimately, I foresee a time when even the bench chemist regularly uses computations in determining the solution to a chemical problem," Golab says. "That is when the computer will finally be accepted as just another tool in the chemist's bag of tricks." ▲

Sabelli rethinks the teaching of chemistry

by Kathleen Robinson, Science Writer

Nora Sabelli. (Photo by John Melchi, Public Information Intern.)

"If I had studied chemistry the way it is taught now, I don't know if I'd have become a chemist. Current teaching methods appeal to people with a specific kind of innate analytical ability. Look at textbooks today—they talk about orbitals and hybridization. I don't think in those terms. I think of the chemistry that needs to be, and then I pick this model when it's useful. To talk about *hybridization* and *orbitals* and never mention the fact that things happen this way because there are energy exchanges—it's absurd. Students are right in not accepting it."

Nora Sabelli, senior research scientist and assistant director for education at NCSA, is reflecting on her personal scientific odyssey. An associate professor of chemistry at the University of Illinois at Chicago (UIC), she divides her time between two responsibilities.

One of her many projects is the development of modules to help students develop an intuitive understanding for chemistry concepts without emphasizing—at the outset—the underlying mathematics. "When the ideas make sense, then people are much more inclined to work at understanding the math. The mathematics is very practical that way. With tools like *Mathematica* [software] and with micro[computer]s widely available, we can rethink the way we teach science."

Encouraging high-performance computing

At NCSA Sabelli encourages established scientists and engineers to include high-performance computational techniques in their research and teaching and to have access to NCSA's Cray high-performance computers in the courses they teach. She does this by one-on-one consulting and by organizing workshops such as the 12-day NSF Workshop on Supercomputing Education held at NCSA in 1989 [see ***access***, September–October 1989] and the 5-day Molecular Dynamics Workshop held in 1990 [see ***access***, July–August 1990]. Sabelli and two

***Sabelli** continued on page 8*

From 10 to 10,000 atoms: computing very large systems

by Kathleen Robinson, Science Writer

With an NCSA CRAY-2 system allocation of 875 hours, Jan Almlöf, professor of chemistry at the University of Minnesota and a researcher at the Minnesota Supercomputer Center, is a major user of NCSA's facilities. A leader in the field of computational chemistry, Almlöf has been working to develop ab initio methods for characterizing the electronic structure of molecules.

Says Almlöf, "What [ab initio] has come to mean in science is that we do not introduce any experimental quantities into our calculations—we do it all from the basic laws of physics that describe the motion of the elementary particles that form the molecule."

Current efforts in computational chemistry are focused on finding ways to enable the study of "extended" systems. Until recently, the largest systems that could be studied with ab initio techniques had no more than about 30 heavy atoms. Almlöf and other chemists now are dealing with systems of about 100 atoms. They hope that within a few years it will be possible to handle polypeptides and other biomolecules, many of which contain tens of thousands of atoms.

The quantum quandary

Starting in the late 1960s, the primary bottleneck for computational chemistry was limited CPU power. Algorithms and computational methods were designed to get around this limitation. The most computationally expensive integrals were identified and kept in memory or on disk. Small integrals and larger ones that were not critical were ignored in the interest of efficiency. The remaining integrals were recomputed only as needed.

As CPUs became more powerful during the 1980s, larger systems could be studied. The increased number of possible arrangements of system components caused memory and disk access to become the hurdles. Says Almlöf, "The algorithms that had been developed to avoid so much CPU work by storing and recycling the data were no longer efficient. It became necessary to minimize the amount of data to be stored on external disk, even at the expense of more CPU work." Working with Almlöf on methods to minimize disk storage is Martin Feyereisen, a postdoctoral computational chemist at the University of Utah.

A basic assumption in years past was that the models describing the quantum behavior of small systems should be valid for larger molecules. Because the necessary calculations are so complex, this assumption severely limited the size of systems that could be studied, Almlöf explains.

"When we made quantum calculations on a system having n atoms, the amount of work we needed to do typically scaled as n^4. If we wanted to double the size of the system we were considering, we had to do 16 times more work. That was a very disappointing fact about the quantum method—it seemed as if we were banging our heads against a brick wall."

Quantum leaps with classical methodology

Recent work done by Almlöf and Itai Panas (postdoctoral computational chemist at the University of Minnesota) has shown that the quantum model is not necessary for many of the interactions in extended systems. "Now that we can study larger and larger systems, we find that a lot of the interactions no longer appear quantum mechanical," Almlöf explains. "It is possible to describe long-range interactions using classical mechanics. That means we can introduce a number of very significant simplifications into the calculation. This is something we have realized quite recently. I think we are only seeing the tip of the iceberg, and it's an exciting development."

Almlöf emphasizes that the simplifications he speaks of are not merely additional approximations. "We are not simply treating the system as a classical one and ignoring all quantum effects. On the contrary—we are systematically monitoring whether quantum effects make any difference. And for many long-range interactions, they don't seem to matter. We don't need to evaluate them if we organize the calculation in an intelligent way."

The difference this makes for the calculations is dramatic: instead of scaling to the power of 4—or even only 2 as was reported just 18 months ago [see ***access***, July–August 1989]—the amount of work needed seems to be roughly linear. Says Almlöf, "When we double the size of the system, we only double the amount of work required to compute it. This, of course, opens a lot of new doors."

Relying on Cray memory

Almlöf cites the CRAY-2 system as "absolutely essential" to this type of work. "At least until recently," he says, "that has been the only machine that provided the necessary memory to carry out these very big calculations."

Although the CRAY-2 high-performance computer was needed to investigate the applicability of quantum mechanics to extended systems, the irony is that the simplified calculations which result from that work can be carried out on super workstations. This does not mean, however, that there is no role for the large machines. Almlöf does not want to see a repeat of what happened in the late 1970s when VAXes became affordable for individual labs. When funding for computer centers was diverted, he says, "that did a lot of damage to the field. Later when much more expensive and powerful machines were developed, in many places there was no organizational structure to acquire and run a supercomputer. I think there will always be a need to push methods and to push the development; that requires the very largest possible computational facility. No matter how powerful a workstation may be, there will certainly be a much more powerful piece of hardware that only a center [like NCSA] can afford." ▲

Sabelli *continued from page 6*

colleagues (Ann Solem of Los Alamos National Laboratory and Steve Roy of UIC) just recently presented a tutorial at Supercomputing '90 entitled "Education and Technology Transfer: A Training Program for Scientific Supercomputing Users."

NSF's mission to bring supercomputing resources and awareness to the academic community extends quite naturally to educating the next generation. Under Sabelli's leadership and in collaboration with other centers, schools, colleges, and universities, NCSA is helping develop curriculum modules. Sabelli is particularly interested in science and engineering outreach to cultural minorities.

Sabelli's personal motivation is not necessarily to train the next generation of computational chemists but to see that scientific methods are understood and accepted by ordinary people. "This is a society based on information," she says, "and access to information is access to control. I am not comfortable with small groups controlling things. I believe in *people.* I don't believe in self-selected groups who know more or can *do* more—it's very dangerous." Her attitude is based, in part, on personal experience.

Integrating chemistry and mathematics

Sabelli's decision to become a theoretical chemist was not merely personal. In 1958 a group of dedicated students in Argentina decided what topics they needed to study abroad so they could work as a team upon their return to South America. "Basically, besides the fact that I had always liked organic chemistry and mathematics," Sabelli explains, "there was a need for somebody to tie together the two areas, and that person was me."

Sabelli received funding to work with theoretical organic chemist Michael Dewar at the University of London. But before she left for England, Dewar informed Sabelli that he was taking a position at the University of Chicago. She changed her travel plans accordingly. For her thesis, she worked on semiempirical methods to calculate properties of aromatic compounds. She remembers cumbersome, hand-cranked mechanical calculators as a limiting factor on early computational research. "I don't even want to remember those methods," she says with a wince.

Returning to Argentina, Sabelli presented her thesis work and received a doctorate. After struggling through several years of political unrest that took a terrible toll on the universities, she and most of her friends had to postpone their hopes of rebuilding the academic community. Sabelli returned to the University of Chicago, where she took "one of those nondescript research positions that young people are offered, and started modifying programs written in assembler." She goes on to explain that her task was incorporating into the calculation how the motion of one electron correlates with the motion of other electrons. Thus began the computing side of Sabelli's scientific career.

In the mid-1960s Sabelli took a position at the UIC computer center. There she turned her unique perspective as a scientist/programmer to advantage in teaching programmers how to work with researchers. She also taught other scientists how to use computers in their research. Sabelli's work led to the development of a quarter-long course for scientific and engineering graduate students in supercomputing use. That course served as the basis for the 10-week version sponsored by IBM and CRI that UIC has continued for several years [see ***access***, May–June 1988]. In 1989 Sabelli accepted a position at NCSA [see ***access***, May–June 1989].

A delicate balance

Maintaining a balance between her computational chemistry research and the demands of teaching scientific computing has been difficult, Sabelli concedes. Strong collaborative relationships have sustained her work when competing demands made it difficult to maintain a normal research schedule. Since the early 1980s, she and Eric Gislason of UIC have been working on the dynamics of negative resonances (unstable states of matter). Gislason, UIC professor of chemistry, investigates reaction dynamics, and Sabelli works on electronic structure. "Between us, we have developed a technique that seems to have a lot of promise," says Sabelli. Working with Sabelli on this project is Linda McDonald, NCSA specialist in education and University of Oklahoma graduate student who teaches physics at North Park College, Chicago [see ***access***, November–December 1989].

In another collaboration at UIC, Victoria Buch-Elder (formerly of the Harvard-Smithsonian Astrophysics Observatory and now assistant professor of chemistry at UIC) is investigating structures such as ice crystals that can be found in interstellar space. "To explain the reactions by which those things decay or evolve," says Sabelli, "she needs to do electronic structure calculations. And that's where we collaborate."

Sabelli also maintains close ties with colleagues at the University of Buenos Aires who are working on ionic crystals. Although she does not consider herself an expert on that topic, she is glad to add her computational expertise to the effort. One of her former students comes for working visits periodically, and Sabelli goes to Argentina to work from time to time.

Transferring knowledge

"Education is *not* something you put on the outside of everything else—it is much more than teaching courses," Sabelli believes. "A teacher is a proselytizer," she adds. "There is no way you can teach something well that you do not believe in."

Although she is sometimes frustrated by resource limitations that hamper important projects, Sabelli nonetheless is positive about her current role. "*All* of NCSA is an educational place—and most people here recognize that. Methodology transfer happens at absolutely every level. It's educational for the people working here and for the outside world. In some sense, we are all educators—we just have different communities, different groups. I find it very exciting." ▲

Lauterbur honored for medical imaging technique

by Jarrett Cohen, Public Information Specialist

About 20 years ago, Paul Lauterbur found that the principles of nuclear magnetic resonance (NMR) could be used to make images, a discovery that has since exploded into a diagnostic technique used in hundreds of hospitals around the world.

For his pioneering efforts, Lauterbur, currently director of UIUC's Biomedical Magnetic Resonance Laboratory (BMRL), has been awarded numerous prizes, including the National Medal of Science in 1987. Most recently, he received the first-ever Bower Award from Philadelphia's Franklin Institute. Carrying a monetary award of $290,000, it is the largest science prize given in the U.S.

"The model was to find someone in this generation who bears a resemblance to Benjamin Franklin," says Charles F. Penniman, Jr., secretary of the institute's Committee on Science and the Arts. It is "given in recognition of outstanding achievement in the life or physical sciences." In 1988, Henry Bower, a Philadelphia chemical manufacturer, bequeathed $7.5 million to the institute to establish the award.

A panel of five "leaders of the world science community" chose Lauterbur from over 100 nominees worldwide, says Larry Tise, director of the Benjamin Franklin Memorial.

Lauterbur is also a Center for Advanced Study professor of medical information science, chemistry, biophysics, and bioengineering at UIUC and Distinguished University Professor of the College of Medicine at UIC.

The discovery

NMR had been used since the 1940s as "a measurement tool in the study of matter, from solid state to chemical compounds to biochemical molecules," Lauterbur says.

While on the faculty at the State University of New York (SUNY) at Stony Brook (after earning a Ph.D. in chemistry from the University of Pittsburgh in 1962), Lauterbur first hypothesized that NMR could be used to make images.

"It occurred to me in 1971, as a consequence of observing NMR properties of tissues taken from rats, that a way to measure the NMR properties of tissue without taking it out and putting it into a test tube was needed," he says.

In NMR imaging, the subject is placed into a magnet, which lines up the atomic nuclei (typically those of hydrogen) contained in tissue. The shape of the magnetic field is then adjusted to tune nuclei in different locations to different resonant frequencies. Small magnetic fields oscillating at radio frequencies are then used to rotate the nuclei out of this alignment. As the nuclei return to their original alignments, a radio signal is produced, which is in turn processed electronically into images.

Lauterbur points out that the basic purpose of using NMR to examine tissue was not new, "but what made the difference was spatial resolution—telling the difference between the signals coming from one organ and another."

Paul Lauterbur in the Biomedical Magnetic Resonance Laboratory. (Photo by John Melchi, Public Information Intern.)

Growth of the field

"After making the first images myself, I continued with undergraduates, who were not yet wise enough to avoid getting involved in something so crazy," Lauterbur says. "One computer programmer was a sophomore." After his initial work, Lauterbur and his students proceeded on a course to help make NMR imaging a practical diagnostic tool.

He began this work using a magnet that had already been used for chemical NMR spectroscopy. At this point, he could study objects 5 mm in diameter. As more advanced instruments were developed, the size of objects he and his students studied grew to 3 cm. Later magnets with inner diameters of 42 cm, and then 62 cm, which can encompass the shoulders and body of an average human being, were obtained.

Through the 1970s, NMR imaging became a worldwide effort, Lauterbur says.

"We were perfecting the techniques on a smaller scale—to define the requirements for larger magnets and how they might be built and used," he says. "Other people also began building whole-body magnets at that time. We didn't regard it as a race, but as a process of developing a collection of ideas, accessories, and techniques. Making magnets bigger was only a part of this."

By around 1980, it was clear that NMR imaging could be routinely useful. Magnets now have openings up to 1 m in diameter, taking in the whole body. Today, there are over

***Lauterbur** continued on page 10*

***Lauterbur** continued from page 9*

2,000 NMR imaging devices in use in the U.S., and over 3,000 worldwide. Thousands of papers about the technique are published each year.

Current developments

Since NMR imaging (usually called *MRI* by radiologists) provides more subtle detail than the x-ray–based CAT scanning, it has come to be the method of choice for studying the head, spine, and (increasingly) the pelvic region and the arms and legs, Lauterbur says.

"Gradually, as better methods have been developed to compensate for motions, it has become more effective in studies of the chest and abdomen," he adds. "The images are either made very rapidly or more complicated methods and computer programs are used to remove the effects of motion."

Magnet design has taken several directions, ranging from the less expensive low-field magnets to the high-end superconducting magnets. This latter class range in strength from 1.5 tesla in clinical systems to 4 tesla in a few experimental systems. (A tesla is the International System unit of magnetic flux density. One telsa equals 10,000 gauss, or about 20,000 times the magnetic field strength of the Earth.) Lauterbur says that the 4-tesla machines are not expected to be routine devices anytime soon and will only be located at special research institutions. "We are hoping to get one," he says with anticipation.

"Our work is not clinically oriented," Lauterbur stresses, referring to the research at his UIUC laboratory. Continuing in the tradition begun at Stony Brook, the BMRL teams are investigating new ideas and better techniques [see ***access***, March 1990].

Zhi-Pei Liang, an NCSA postdoctoral research associate, is working with BMRL on a new way to do spectral localization, a method of "finding where signals from particular compounds come from," Lauterbur says [see ***access***, September–October 1990]. While hydrogen nuclei, especially in water, are the most common target of study, NMR signals of less abundant phosphorous and carbon nuclei in physiologically important compounds are also analyzed. Liang is developing algorithms to observe and measure them more clearly than has been possible previously. "Because nuclei in different molecules have different frequencies, we can find the concentrations of molecules and identify them in tissue," Lauterbur says.

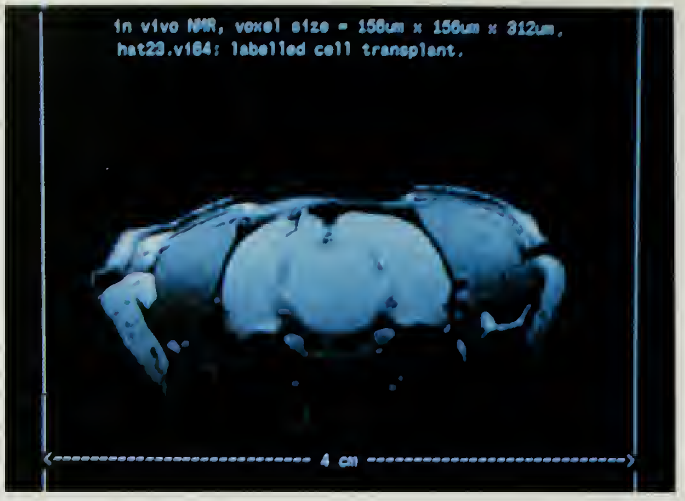

in vivo NMR, voxel size = 156um x 156um x 312um,
hat23.v184: labelled cell transplant.
4 cm

Image from an NMR dataset of a live rat brain transplanted with iron oxide-labeled cells. Dark areas in upper left correspond to labeled cells at the injection site. (Dataset processed on NCSA's CRAY-2.) (Photo courtesy of Pratik Ghosh, Biomedical Magnetic Resonance Laboratory.)

Another field of investigation at BMRL is NMR microscopy, which involves making images of small objects or of smaller regions of large objects. Lauterbur says that they can get a resolution of 10 micrometers, about the diameter of a single cell. Microscopy research also includes comparing NMR images with optical images.

Tagging cells and tissues with magnetic molecules and particles is a fairly new technique in NMR imaging. "The clinical world calls these *contrast agents*," Lauterbur says. Tagged cells and tissues change the NMR properties of the water in a tumor or organ and often reveal differences that would otherwise have been missed.

"We are interested not only in the ultimate clinical use of tags for certain kinds of cells but also in synthesizing new kinds of molecules that may be used in different ways," Lauterbur says.

One application, now in the early stages, is labeling brain cells from a rat with magnetic particles and transplanting them into the brain of another rat. This work is being carried out in collaboration with William Greenough's laboratory at UIUC's Beckman Institute. It may help determine where transplanted cells go in the brain—information critical to their use for studying brain function and treating human disease.

According to Greenough, the initial goal of this work was to develop methods of evaluating transplant stability in animal models for disorders such as Parkinsonism. Additional spin-offs include possible methods for analyzing the brain's repair processes and for diagnosing certain disorders involving brain vascular failure.

Greenough, an NCSA principal investigator, is associate director of the Beckman Institute and a UIUC professor of psychology.

The role of supercomputers

NMR scans produce large amounts of three-dimensional data, or even four-dimensional data, which are often best handled by a supercomputer. BMRL's NMR machine is connected to NCSA's CRAY-2 supercomputer by a fiber optic connection, and the laboratory uses several hundred hours of time each year.

"Our image reconstruction methods are very computer intensive, and they would not be practical with the instrument computer system here," Lauterbur says. "Some of the work is best done in a real-time mode, or close to it."

In addition, three-dimensional visualization is an effective way to display complex images, Lauterbur says. Clint Potter, on the BMRL staff as well as an NCSA research programmer and head of NCSA's biomedical imaging applications team, and NCSA's Visualization Services and Development group have been instrumental in this area, he says.

"With NCSA, we can get a jump on the field," Lauterbur says. "If we find that the best or only practical way to do an experiment requires supercomputer processing, we don't have to give up," he adds. "We do them in the best way we know how, using NCSA facili-

***Lauterbur** continued on page 16*

Computational chemistry allocations

by Patricia Wenzel, Manager, Client Administration

Research projects in computational chemistry that are currently underway at NCSA are as follows:

Jan Almlöf, U. of Minnesota at Minneapolis, *Development and Applications of Direct Methods for Electronic Structure Calculations.*

Roger Anderson, U. of California at Santa Cruz, *Synthesis of Diffraction Patterns for Large Random Fractal Aggregate Clusters.*

Robert William Armstrong, California State U. at Los Angeles, *Theory and Modeling of Organic Reactions and Stereoselectivity.*

R. Stephen Berry, U. of Chicago, *Chaotic and Ergodic Properties of Clusters: A Subtopic of Few Body Dynamics of Atoms and Molecules; Few Body Dynamics in Atoms, Molecules, and Clusters.*

George Blyholder, U. of Arkansas at Fayetteville, *Catalytic Reactions on Transition Metal Clusters.*

Thomas David Bouman, Southern Illinois U. at Edwardsville, *Linear Response Calculations of Molecular Properties.*

David Brant, U. of California at Irvine, *Conformational Dynamics of Oligosaccharides.*

Kevin Burgess, Rice U., *Molecular Orbital Calculations and the Ceiplak Effect.**

Lonnie Dean Burke, UIUC, *Conformational Isomerism of Substituted Azomethine Ylides.*

Ngee Sing Chong, Rice U., *Molecular Modeling of Chemisorption of Corrosion Inhibitors (Aniline Derivatives) on Iron Metal Surface.**

David Coker, Boston U., *Development of Simulation Methods to Study Nonadiabatic Nuclear Dynamics of Solvated Electron Systems.*

Zareh Darakjian, Rice U., *Quantum Theory of Reactive Scattering.**

Ernest Davidson, Indiana U., *Molecular Interactions.*

Carol Deakyne, Eastern Illinois U., *Lewis Acidities of SO(3) vs. BF(3).**

John Delos, College of William and Mary, *Excited States of Atoms.*

Dana Dlott, UIUC, *Vibrational Heating by Shock Wave.*

Anthony Duben, Southeast Missouri State U., *Spectral Density Functions: Anisotropic Motion.**

Carmen Giunta, LeMoyne College, *Kinetic Modeling of the Chemical Vapor Deposition of Fluorine-Doped Tin Oxide Films from Dimethyltin Dichloride, Oxygen, and Trifluoromethyl Bromide.*

Joseph Golab, UIUC, *Theoretical Investigations of the Surface Enhancement Effect: Calculations on Ag-Pyridine Cluster Compounds.*

Mark Gordon, North Dakota State U., *Potential Energy Surfaces and Dynamics for Reactions of Bicyclobutanes.*

A. D. J. Haymet, U. of Utah, *Chemistry.*

Warren Hehre, U. of California at Irvine, *Development and Parameterization of Intermolecular Potentials for Molecular Dynamics and Monte Carlo Simulations.*

Mark Hoffman, U. of North Dakota, *EPSCOR-Chemistry.*

Detlef Hohl, UIUC, *Molecular Dynamics and Density Functional Theory: Static and Dynamical Properties of Main Group V and VI Clusters, Liquids, and Amorphous Solids.*

Andrew Joseph Holder, U. of Missouri at Kansas City, *An Electronic/Molecular Structure Correlation for* $H_2Fe(CO)_4$ *and Derivatives (Revised); A Speed Comparison of MOPAC and AMPAC; Semiempirical and (Ab Initio) Investigation of the Homotropylium Cation Potential Energy Surface.*

Anton Hopfinger, UIC, *Molecular Dynamics of Order-Order Phase Transitions in Chain-Molecules.*

Werner Horsthemke, Southern Methodist U., *Heterogeneous Nonlinear Chemistry.**

Martin Karplus, Harvard U., *Free-Energy Simulations on Biomolecules; Theoretical Study of Lambda-Repressor-DNA Complex; Vibrational Contributions to Biomolecular Phenomena.*

Peter Langhoff, Indiana U., *Molecular Photochemistry and Physics.*

Pierre LeBreton, UIC, *Photoemission Scaling of Nucleotide Valence Orbital Structures: Factors which Influence Electrophilic Attack of DNA.*

Gilbert Mains, Oklahoma State U., *Isomerization Barriers in Substituted Anisoles.*

James Andrew McCammon, U. of Houston at University Park, *Theory of Biomolecular Structure and Dynamics.*

Dwayne Miller, U. of Rochester, *Transport of Electronic Energy in Disordered Systems.**

William Miller, U. of California at Berkeley, *Quantum Reactive Scattering.*

John Nicholas, UIC, *Molecular Dynamics Simulation of Silicalite.*

Andrzej Rajca, Kansas State U., *Highly-Charged He/C Clusters: Hypervalent Carbon.*

George Schatz, Northwestern U., *Theoretical Studies of State-to-State Chemistry.*

Don Secrest, UIUC, *Complex Collision Processes.*

Harrell Sellers, UIUC, *Electronic States of Chromium Hexacarbonyl; Transition Metal Chemistry-Catalysis.*

Rex Skodje, U. of Colorado at Boulder, *The Quantum Phase Space Hydrodynamic Model for Studying Transport and Chemical Reactivity.*

Jean Standard, U. of Oregon, *Potential Energy Surfaces Using the Bootstrap Method.**

Christos George Takoudis, Purdue U., *Rate Constants of Gas Phase and Surface Reactions.**

Almon Turner, U. of Detroit, *Role of* $Cl\text{-}NO_x$, $F\text{-}NO_x$ *Type Molecules in Ozone Depletion.*

Peter Wolynes, UIUC, *Nonequilibrium Statistical Mechanics: Tertiary Structure Recognition Using Associative Memory Polymer Hamiltonians.*

Bernhard Wunderlich, U. of Tennessee at Knoxville, *Theoretical Studies of the Dynamics and Structure of Macromolecules.*

Robert Wyatt, U. of Texas at Austin, *Quantum Reactive Scattering via the Log-Derivative Version of the Kohn.*

Chong Zheng, Northern Illinois U., *Simulation of Solid State Reactions.**

*Allocations made through NCSA's Affiliates Program.

For details about how to apply for time on NCSA's high-performance computers, contact Patricia Wenzel, manager of Client Administration [see **NCSA contacts**, page 15.] ▲

Newsletter survey results

by Fran Bond, ***access*** *Editor, and Stephanie Drake,* ***data link*** *Editor, Information and Publications Division*

Responses to the ***access*** and ***data link*** readership survey poured in from mid-May through mid-June. Thank you so much for replying. So many of you responded that we were still tabulating and analyzing the results after the deadline [see ***access***, July–August 1990].

According to media experts, it is unusual for more than 5% in any group surveyed via U.S. mail to respond. As of June 15, our readerships had overwhelmed that statistic with an 11% response rate as follows:

	U.S.	**UIUC**	**Total**
surveys mailed	4,782	1,203	5,985
surveys returned	513	157	670

The following significant points resulted from the survey:

- Two-thirds of the respondents were NCSA users; one-third were nonusers. (Academic scientists/researchers, graduate/postdoctoral students, and industrial scientists/researchers were the top three communities responding.)
- Our readership reflects a wide diversity of interests—over 170 areas.
- Almost 80% of the respondents read both newsletters.

Sections of ***access*** that were ranked as the most useful (in order of preference) were the following: Software applications, Science and research [now Research] and NCSA-developed software tied for second, and NCSA contacts was third. Readers found these sections so useful they wanted more coverage of NCSA-developed software, Science and research, Software applications, Visualization, and NCSA contacts (in that order).

Among the suggested features that might be added to ***access***, the most popular was for "articles on trends in the supercomputing industry and computational science." Second was "guest articles," with "more technical information" placing third.

Most respondents found ***data link*** useful: 80% consult it between issues. Readers asked for more details and more examples; periodic coverage of basics for new users; and additional information on software, both commercial and NCSA-developed packages.

We keep publication costs down by printing on standard paper purchased in large quantity by UIUC, by keeping our computerized mailing list current, and by mailing at bulk postage rates. For some time ***data link*** has been printed on recycled paper, and we are working with our printer regarding recycled or recyclable paper for publications illustrated in color.

Through both newsletters, NCSA keeps its users and the public informed of advancements in high-performance computing. Feel free to get in touch with us at any time by contacting the Publications Manager [see **NCSA contacts**, page 15].

Thanks again for taking the time to send us your valuable comments. ▲

CRAY Y-MP4 installed

According to Sue Lewis, manager of NCSA's Central Facility, hardware installation of the Y-MP is completed and software installation is finished as we go to press. As of October 25, the machine was available for staff logins. The Y-MP system became available for full production November 5. (Photo by Vincent Jurgens, NCSA Media Services.)

Fall events at NCSA

Counterclockwise from above right: At UIUC's CompuFair90, NCSA's exhibit attracts many onlookers. (Photo by John Melchi, Public Information Intern.) • At the Beckman Institute Open House, Benno Puetz explains a robotic study of the Theoretical Biophysics Group. (Photo by Fran Bond, Publications Editor.) • At the Affiliate Representative Meeting recently hosted by NCSA, Dave McWilliams (left), NCSA academic affiliates coordinator, answers questions about NCSA-produced software for Timothy Hardy (right), University of Northern Iowa affiliate representative. (Photo by Tony Baylis, NCSA Media Services.) • NCSA Director Larry Smarr (left) gives NSF's Tom Weber (right), director of the Advanced Scientific Computing Division, a tour of the Machine Room during renovation. (Photo by Tony Baylis, NCSA Media Services.) • At the Computational Science and Education NSF Workshop, participants tour the training facilities. Jean Shuler (center), Los Alamos National Laboratory, discusses NCSA's systems with NCSA research programmer Crystal Shaw (right) while Al Rogers (left), FrEdMail Foundation, tries a graphics application. (Photo by Cordelia Baron, NCSA Media Services.) ▲

Lilly FOCUS

Eli Lilly and Company's "FOCUS III," intensive workshop on research applications, was held at NCSA for a week at mid-September in which 27 Lilly staff members participated. Attendees are pictured above with Riaz Abdulla (second row, right), head of Lilly's Supercomputer Applications and Molecular Design Department. (Photo by Wilmer Zehr.)

Tentative training dates: 1991*

January 14–16	Cray Applications Training**
February 18–22	Cray Code Development Training
March 18–22	Connection Machine (CM-2) Training
April 15–17	Cray Applications Training
April 29–May 3	Affiliates Training
May 13–17	Cray Code Development Training
June 17–19	Connection Machine Training
August 19–23	Cray Code Development Training
September 16–18	Cray Applications Training**
September 30–October 4	Affiliates Training
October 14–18	Cray Code Development Training
November 11–15	Connection Machine Advanced Training
December 9–11	Cray Applications Training**

You must register to attend NCSA training. Class size is limited.

To register Contact Training Program Registration [see **NCSA contacts**, page 15]. Industrial partner users, contact your representative at NCSA.

For additional information Contact the Training Program [see **NCSA contacts**, page 15].

*Dates and topics are subject to change.

**Applications will be in the fields of chemistry, finite element analysis, and computational fluid dynamics.

Computational catalysis *continued from page 4*

the RS/6000 saturated. We find that this works well for us."

In one project, Sellers is collaborating with Roger Ove, NCSA research scientist and UIUC adjunct assistant professor of mathematics and astronomy. Sellers and Ove proposed chemical explanations for the now-debunked cold fusion experiment. "One of the useful things that came out of the cold fusion fiasco was the notion that there probably is chemistry taking place in the *interstitial* (interior) regions of poorly prepared metal crystals."

Using the CRAY-2 and the IBM RS/6000 systems, Sellers developed an animation to look at alternatives to the cold fusion claim. "What we found in this series of calculations is that the hydrogen molecule inside the palladium crystal dissociates and bonds to the metal atoms forming (chemically) palladium hydride. There is no hydrogen molecule anymore. What we get are two palladium hydrides. One of our ideas is that any heat production observed could come from a chemical reaction such as the formation of palladium hydride, or a reaction between the hydrogen and the oxygen that may also be trapped inside the crystal. Also, the formation of the palladium hydride would weaken the crystal lattice and actually help propagate cracks that would increase the formation of the hydride. So you could have little bursts of runaway chemical reactions taking place."

Looking ahead

Sellers envisions a day when catalysts will be fully understood which could result in tremendous advances in pharmaceutical and chemical development, and when engineered coatings would have removed the threat of rejection for those needing artificial implants.

"We're already to the point where, given enough time and high-performance computing hours, we can make some very accurate predictions about a reaction mechanism. That is a tremendous accomplishment, and it's just the beginning." ▲

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Lauterbur *continued from page 10*

ties, and expect computer technology to catch up in the next few years. It will then be possible to do the necessary computations on a desktop.

"We can plan ahead in this way, and influence the development of new instruments and methodology for future years and advanced applications." ▲

NCSA Reformat, a new utility

by Peter Webb, Programmer, Software Tools Group

Many of the utilities developed at NCSA read and write HDF (Hierarchical Data Format) files. (HDF, produced by NCSA's Software Tools Group, provides a multiobject file format for transferring graphical and floating-point data among several platforms.) Since HDF is not the only file format used for the storage and transmission of scientific data and images, there is a vast amount of data stored in formats that is incompatible with those utilities. **NCSA Reformat** makes more of that data available by converting it to HDF. Currently, the conversion of 8-bit images (RI8 sets) and scientific data (where present) is supported by the new utility.

NCSA Reformat recognizes the following file types: GIF, TIFF, FITS, Sun raster, and X window dump. This code was developed on a Sun Workstation and has been tested on the SGI Personal IRIS workstation, the Stellar, and the CRAY-2 system.

For further details about this new NCSA-developed product, see "NCSA Reformat—a file-conversion utility" in the current issue of ***data link***.

For further information about the utility, contact Peter Webb by telephone at (217) 244-0015 or by electronic mail at pwebb@ncsa.uiuc.edu (Internet) or u26277@ncsagate (BITNET).

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- Hot tips and topics
- Background on the CRAY Y-MP
  by Kurt Hirchert, Team Leader, Consulting Group
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- Good passwords minimize chances of account vandalism
  modification of article by Jeff Smith, UNIX Systems Administrator, Purdue University Computing Center
- NCSA Reformat—a file-conversion utility
  by Peter Webb, Graduate Student Programmer, Software Tools Group

To receive a copy of the current issue of ***data link***, contact the NCSA receptionist at (217) 244-0072.

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This document contains index entries for the 1990 *access* newsletters. The three numbers used for the entries and subentries indicate the volume, issue, and page number(s) of the citation, in that order. For example, 3.4.6–7 means that the entry is in volume 3, issue 4, pages 6–7 of the newsletter.

You can also find this index online in the /usr/local/doc directory on the CRAY Y-MP and CRAY-2 systems. To view the index online, using the UNICOS file pager more, enter:

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Visualization

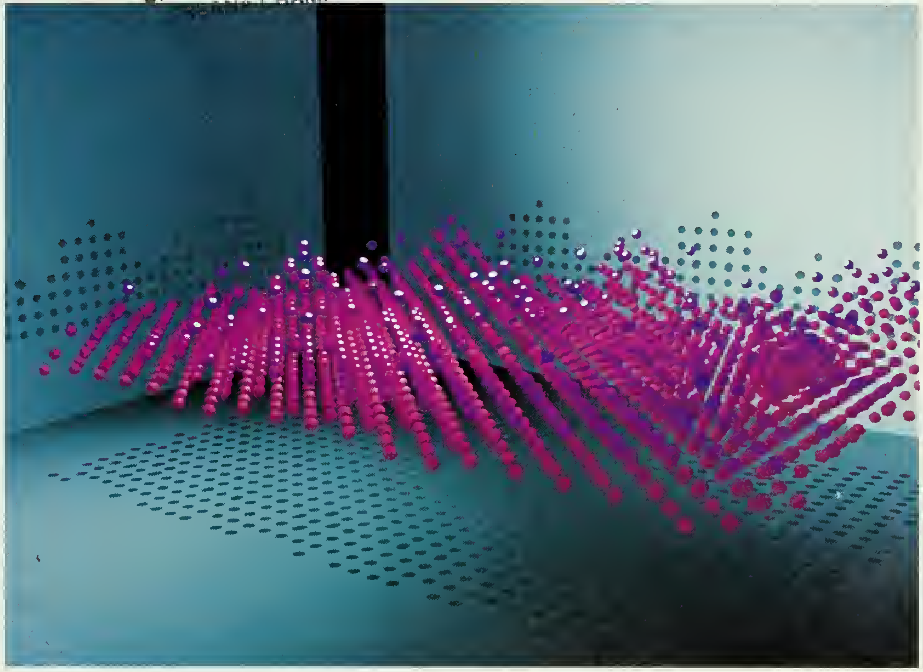
Plasma physicist produces video paper

by William Dwyer,
Graduate Assistant Writer

You may soon hear scientists asking each other, "Have you 'read' a good video paper lately?" David Ruzic, UIUC plasma physicist, recently presented his research findings in video paper format, a new technique to communicate science.

"There's that old saying, 'A picture's worth a thousand words," explains Ruzic, associate professor in the Department of Nuclear Engineering. Ruzic worked with NCSA's Visualization Services and Development (VSD) and Media Services groups to produce a videotape of his research findings in ion–surface interactions. On the videotape of "Hydrogen Collision Dynamics on a Rough Nickel Surface," Ruzic narrates the voice-over while he appears on camera to explain his research.

According to Ruzic, the video paper conveys much more information graphically than the written work possibly could. Ruzic says his video would be as handy to use as a book because the viewer can start at the beginning or at any other point. For those who wish to learn about Ruzic's research and hear him describe it as it is visualized, this video paper will be available like any book or journal. It is referenced in technical papers and *The Handbook of Plasma Processing Technology* (edited by S. Rossnagel, J. Cuomo, and W. Westwood).



Still from introduction to "Hydrogen Collision Dynamics on a Rough Nickel Surface" showing the formation of surface atoms. (Courtesy of NCSA Visualization Services and Development group, pages 1 and 3.)

Challenging semiconductor technology

Ruzic believes that his research in plasma–materials interaction challenges the technology of semiconductor production. Semiconductor chips are made by plasma processing techniques, which require knowledge of the physical properties in plasma–surface interactions. Successes in the field thus far have been through "trial and error." But according to Ruzic, "that's not the way to do science" if one wants to push technology.

In Ruzic's model, an energetic hydrogen atom representing plasma interacts with surface–metal atoms in a cubic lattice. (A *lattice* is a regular periodic arrangement of points in a three-dimensional space.) He used a molecular dynamics program code, the

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Abbreviations

ACM	Association of Computing Machinery
CRI	Cray Research, Inc.
NCSA	National Center for Supercomputing Applications
NSF	National Science Foundation
UIC	University of Illinois at Chicago
UIUC	University of Illinois at Urbana-Champaign

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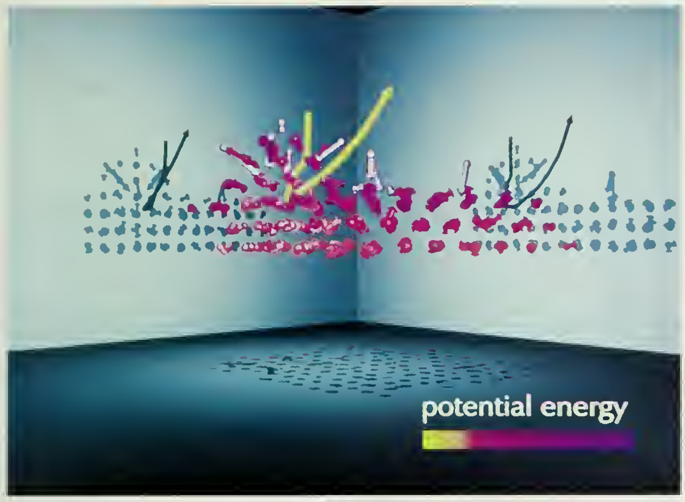
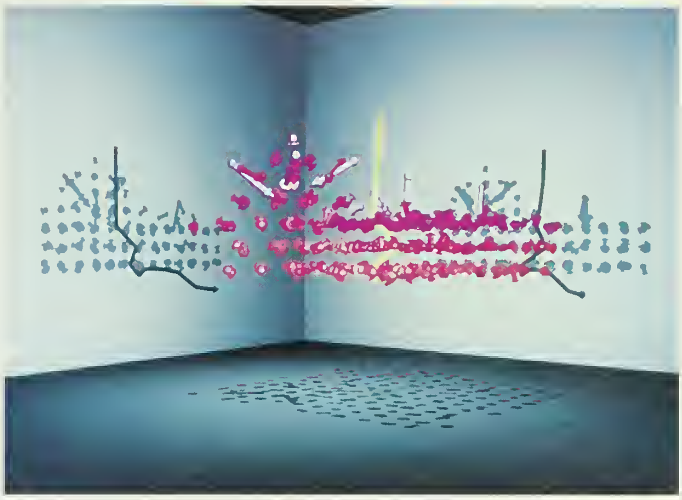




Yellow streamers indicate path of hydrogen atom through a nickel surface to show reflection (top left), absorption (top right), and hover (below right).

Plasma physicist *continued from page 1*

Embedded Atom Method developed at Sandia National Laboratories, that is based on potential energies of atoms. As a hydrogen atom approaches metal atoms in the lattice, potential energies of nearby atoms change, or interact, with the hydrogen atom's energy. Every known quantity was added to the model to study the results of real surface interactions.

To approximate an actual surface, Ruzic used fractal geometry to incorporate surface roughness in the model. While a graduate student at Princeton University, Ruzic heard a lecture by the famous fractal geometrician Benoit Mandelbrot. "I had an idea that using fractals should be the way to model these surfaces," says Ruzic in acknowledgment of Mandelbrot's influence. Ruzic incorporated the fractal model in another code—a binary collision model.

For the plasma–surface simulation, the code calculates energy changes once every femtosecond (*femto* represents 10^{-15}, or one-thousandth of a millionth of a millionth) of real time for 1,000 atoms that interact with a moving hydrogen atom. Such calculations require an "immense amount of resources," Ruzic says—thus the need for supercomputers to perform the simulation. Ruzic first used the CRAY X-MP/48 system for his research. For his work on vacuum technology and plasmas, he received the Xerox Award for Faculty Research last spring.

Visualizing plasma–surface interactions

After developing a suitable model, Ruzic visualized the hydrogen atom's interaction with surface atoms in collaboration with NCSA visualization developers Gautam Mehrotra and Aliza Corson of VSD. Their animated visualization takes viewers on a "ride" with the hydrogen atom.

"Our role here is mainly one of mediation between the data and the final image," explains Mehrotra. He programmed the model so that unit cells of simulated space containing the metal atoms could be stacked together to create an enveloping lattice. His major challenge was matching cells within each frame of a sequence to show the hydrogen atom leaving one cell and then appearing in a neighboring cell as it moved continuously through the lattice.

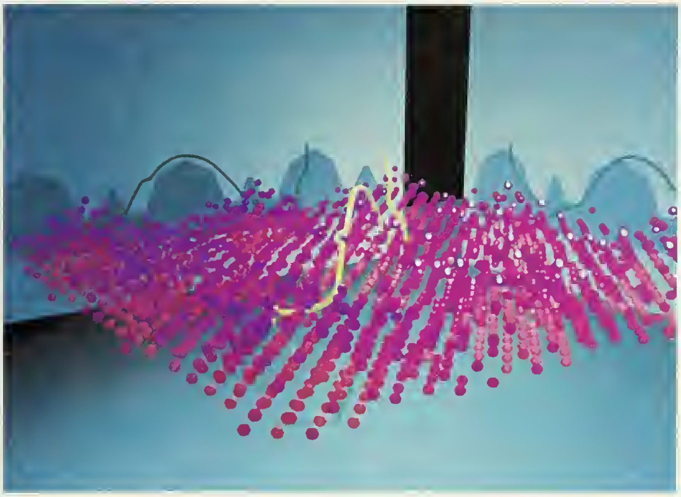
Corson and Mehrotra developed two methods for visualizing energy and motion differentiation in atoms. To represent potential energy changes, atoms are shown as spheres that change color in a spectrum ranging from yellow to purple. Motion, or kinetic energy, is shown by arrows to depict the vectors of motion. An arrow points the direction of an atom's motion; its length indicates the atom's speed.

To orient viewers to the lattice's construction, an introductory sequence shows cells building and forming the lattice. This segment is entitled "Construction of a Nickel Surface Characterized by Fractal Geometry."

Three animated sequences show the hydrogen atom interacting with surface atoms. In the first, the atom bounces off the lattice to represent reflection. In the next, it penetrates the surface of the lattice to show absorption; in a third, it almost reflects and is then drawn back into the surface to represent hover.

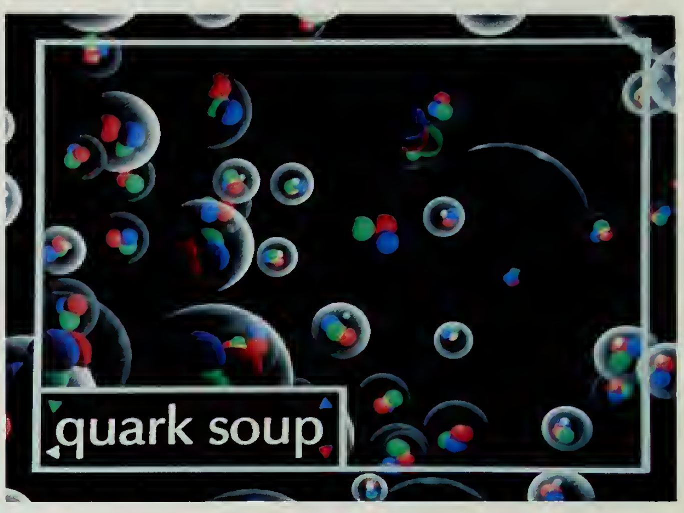
As the hydrogen atom moves through the lattice, the viewer follows behind the atom and scans the structure before zooming in on the hydrogen atom's near-collision course around nickel atoms. Nickel atoms change directions and colors as they interact with the hydrogen atom to illustrate ion–surface interaction.

Plasma physicist *continued on page 18*



SIGGRAPH '90 recap

by Jarrett Cohen,
Public Information Specialist

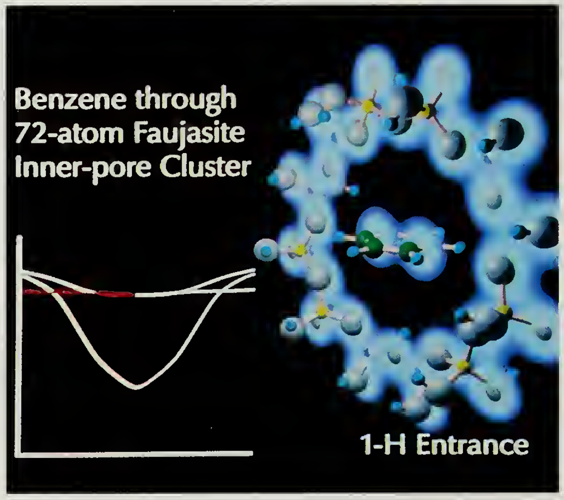


"As a result of computer graphics, this country is experiencing a kind of Renaissance, where we have disciplines coming together," said Donna Cox, NCSA Associate Director for Numerical Laboratory Programs, introducing press attendees to SIGGRAPH '90 in Dallas, TX. "Collaborations not only extend to the scientist working on data representation, but computer graphics are bringing together academia and industry in novel ways—solving problems that have major societal impact."

Cox used the Amoco-NCSA visualization "Computational Quantum Chemistry in Catalysis Research" to exemplify this collaboration. Since catalysis plays a role in many manufacturing processes and is therefore fundamental to the economy, "computer graphics are affecting industry in a major way," she said.

Legislators can also gain insight from graphic techniques, Cox added. Scientific visualization "will shape the future of global environmental issues." Gregory McRae's smog research (see opposite page), for example, will be instrumental in the regulation of automobiles, she said.

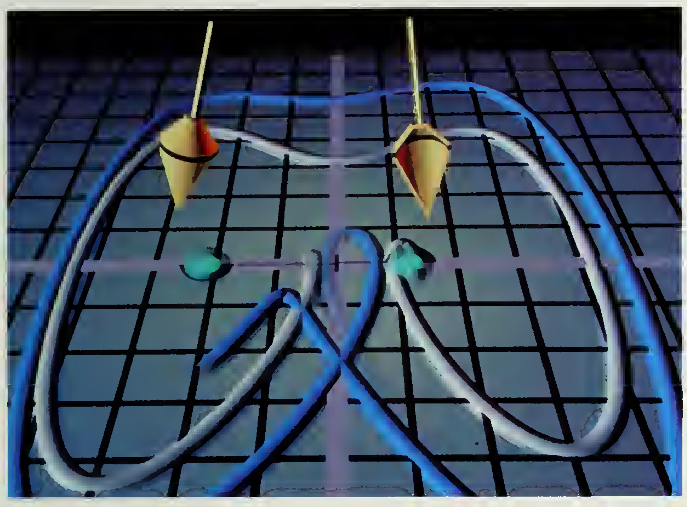
Other speakers at the briefing included Michael Ester, J. Paul Getty Trust; Walter Bender, MIT Media Lab; and Michael Wahrman, deGraf/Wahrman, Inc.



Grand challenges

The "Grand Challenges of Computational Science" panel addressed the top four societal priorities set forth by the Office of Science and Technology Policy of the Bush administration: high-performance computing (HPC), industrial competitiveness, environment and global change, and education. NCSA Director Larry Smarr chaired the panel.

Smarr said that the proposed HPC program would dwarf the NSF supercomputer centers program, whose current annual budget is $50 million. By the beginning



SIGGRAPH '90 entries. On the opposite page, top, "In Search of the Fingerprints of God," (Independent Project); center left, "Computational Quantum Chemistry in Catalysis Research" (produced by NCSA Visualization Services and Development [VSD] group for Amoco); center right, "Under the Puddle" (Independent Project—computations at Ohio State University, postproduction at NCSA); bottom, "Smog: Visualizing the Components" (produced by VSD).

This page, top, "Excerpt from Time Dependent Behavior of Simple Dynamic Systems" (produced by VSD); bottom, "Venus and Milo" (produced by Donna Cox with UIUC, Art Class 331, and NCSA Post Production Facility). [For more information, see *Film and Video Theater: The Pioneers Return to Dallas, SIGGRAPH 1990* (catalog) and ***access***, July–August 1990.]

of federal FY92, the government plans to earmark $150 million in new money for HPC; in FY96, $600 million annually.

Three distinguished scientists joined Smarr to discuss some of the grand challenges which the HPC program will help drive.

Chemistry: David Dixon, research scientist at E.I. Du Pont De Nemours & Co.'s central research laboratory, discussed work on chlorofluorocarbons, chemicals which can attack the Earth's protective ozone layer. Du Pont is using their Cray Research computer system to search for more environmentally benign replacement chemicals. Dixon also described how Du Pont has created computational models for each of the major polymers on which the company's business rests.

Biology: "Computational biology is a different sort of field; it didn't exist 10 years ago," said Eric Lander, a MacArthur fellow at MIT's Whitehead Institute. Now computational techniques are applied to genome analysis, biomolecular sciences, biological systems research, and medical imaging.

Lander's work is part of the Human Genome Project, a multilaboratory effort aimed at eventually creating a map of the human genome—comprised of 3 billion base pairs.

Genome maps are being generated by tracing inheritance patterns of genetic disorders and by directly probing human DNA. Teraflop machines will be necessary to assemble and understand all the resulting sequences, Lander said. "We now only have 1/1000 of the data within the genome project completed," he added. For these smaller fragments, Lander has used NCSA GelReader for the Macintosh as an analysis tool [see ***access***, February 1990; March 1990].

Air pollution: Gregory McRae, professor of chemical engineering and engineering and public policy at Carnegie Mellon University, showed two videos. The research topic was the Los Angeles air pollution problem. The supercomputer simulation was performed at the Pittsburgh Supercomputing Center (PSC), on which McRae reported at an NCSA seminar last December [see ***access***, February 1990]. As a result of that visit, McRae

SIGGRAPH '90 *continued on page 6*

SIGGRAPH '90 continued from page 5

came to NCSA to create "Smog: Visualizing the Components," which appeared in SIGGRAPH '90's Film and Video Theater [see ***access***, July–August 1990]. Taking viewers inside the smog to see the dispersal of noxious particles, this video visualized the amount of pollution produced daily in Los Angeles. A second video was later produced at PSC; it explored three-dimensional patterns of the tropospheric ozone. Already McRae's research has impacted environmental policy in the U.S., and he foresees this type of work having a global influence.

Smarr concluded the panel by articulating a role for computational science in education. NCSA's work in this area has included equipment donations and training support. Networking Champaign-Urbana schools for collaborative projects is also being studied, he said.

One popular topic at SIGGRAPH '90 was virtual reality, which allows a user to manipulate a data space much as s/he would in a real-life architectural environment. "With Nintendo, kids are into virtual reality today. The question is how to create software that will let them apply the skills they are learning to exploring simulations of physical reality," Smarr said.

Advances in visualization

As chair of "Beyond Scientific Visualization: Mapping Information," Cox discussed the variety of techniques recent NCSA visualizations employ. She pointed to the future of scientific visualization by showing how sound complements the visual image (in this instance, the chaotic motion of a pendulum) in "Time Dependent Behavior of Simple Dynamic Systems" by Mark Bajuk, NCSA scientific animator. "We should be thinking not only of visual techniques but others—sensualization," Cox said. "Maybe we are moving toward visceralization," Bajuk added.

Richard Ellson, Eastman Kodak Co., spoke about visualization of plastic injection molding [see ***access***, July–August 1990]. Cameras and typewriter ribbon cases are among the products Kodak produces using this process. Ellson said that a real-time version of the visualization running on Sun Workstations and AT&T Pixel Machines can generate a particular mold simulation in 10 minutes.

CalTech's Mathematics! Project is a series of videotapes designed for use in high schools. Jim Blinn, its director, showed how different colors and shades of a color can be important for indicating position, velocity, and acceleration. He also discussed mathematics textbooks' influence on his videotapes—for example, in using the same type conventions so as not to confuse the viewer.

Donna Cox, associate director of NCSA's Numerical Laboratory Program. (Photo by David Curtis, Information and Publications Group.)

The last panelist of the session, Helga Leonhardt Hendriks, presented a paper on her Leonhardt Language System, which uses visual representations for parts of speech and their interactions with one another. Developed in 1977, a videotape demonstrating the system was made with NCSA in 1988. "The film allows the user to experience language," Hendriks said.

On the Hill

Cox also chaired a panel concerned with federal funding of high-performance computing and computer graphics research, "What is Happening on the Hill?" In her opening remarks, Cox pointed out that the average academic spends 40 percent of his/her time seeking funds.

Smarr addressed the HPC Program with respect to details about where decisions have been made to implement it. "The agencies have agreed beforehand how to spend all the money," Smarr said. He cautioned that the mounting conflict with Iraq could redirect funds to the military.

Rich Hirsh, director of the NSF supercomputer centers program, spoke on NSF's support of visualization, which falls into three areas: generic support, by providing software

***SIGGRAPH '90** continued on page 18*

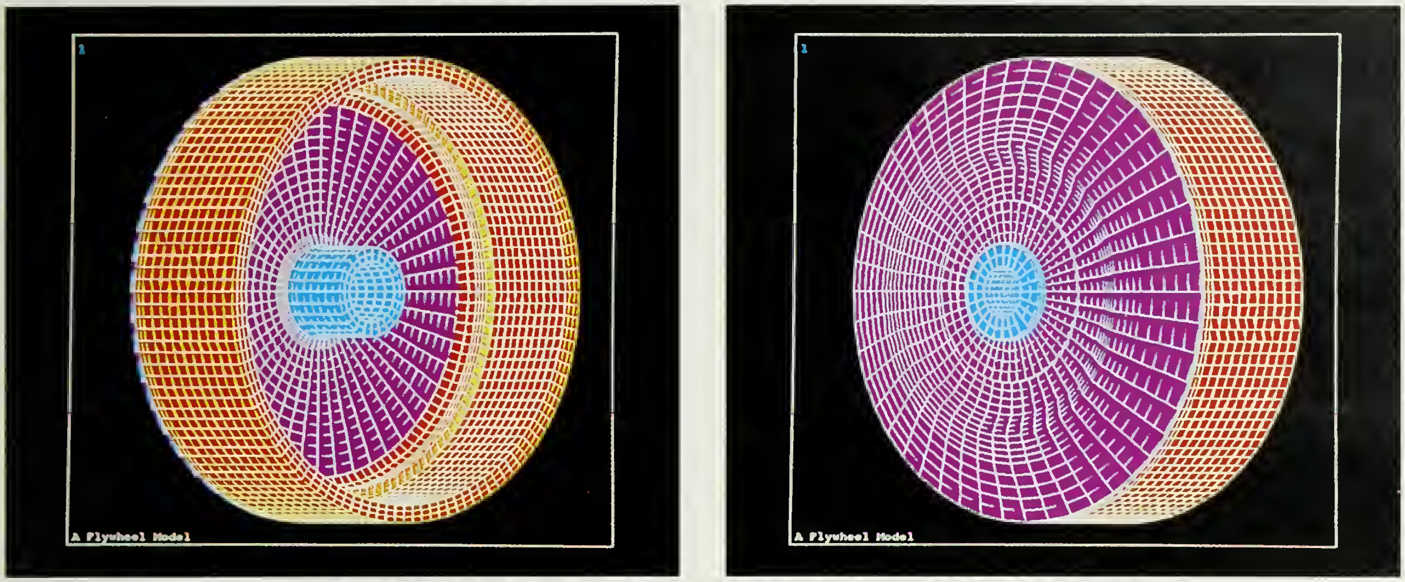
NCSA animations à Paris

Two NCSA-produced scientific animations, "Study of a Numerically Modeled Severe Storm" and "Instabilities in Supersonic Flows," are now on exhibit in France.

Part of a semipermanent computer graphics exhibition at la Villette, or La Cité des Sciences et de l'Industrie, in Paris, they will be shown for at least the next 5 years in the exhibit "L'Image calculée" (literally "Computer Images"). A condensed version of this exhibition will travel to other science museums throughout France.

From September to December 1990, another version is on display at the Centre d'art et de culture Georges-Pompidou, or Centre Pompidou (France's national museum of modern art—commonly called the Beaubourg). NCSA's animations are part of a show illustrating the aesthetic quality of scientific images.

Members of the NCSA staff who worked on the storm animation are Robert Wilhelmson, Harold Brooks, Brian Jewett, Crystal Shaw, and Lou Wicker (science); Matthew Arrott, Mark Bajuk, Colleen Bushell, and Jeffery Yost (animation). Michael Norman (science); Donna Cox (visualization); and Ray Idaszak (animation) produced the animation of supersonic flow. ▲



Model of an engine flywheel using finite-element method. (Courtesy of Fouad Ahmad and Mike Krogh.)

Fouad Ahmad analyzes structures via FE

by Randall Graham, Science Writer

"I entered engineering using a slide rule," recalls Fouad Ahmad. "My first finite-element project involved 100 elements and took hours. I could do the same problem today on a Cray in seconds."

But some of Ahmad's former students did not share his hindsight. "Not long ago I had a student complain to me that the finite-element software he was using on the supercomputer wasn't 'user friendly.' Here's a guy with a 3D model that he can rotate to any angle, and it displays stress contours in full color. That's not user friendly?" Ahmad chuckles, "I told him he was spoiled."

One man, many roles

Ahmad, who came to NCSA in January 1990 as a visiting scientist, has joined the staff as a research scientist. Formerly an assistant professor of engineering mechanics at the University of Wisconsin at Milwaukee, he is a specialist in finite-element (FE) analysis.

While a visitor at NCSA, Ahmad had four primary functions. He is continuing to work in those areas as a full-time staff member. Ahmad evaluates FE codes on the CRAY X-MP/48 and the CRAY-2 systems, teaches a course in NCSA's New User Training Program, conducts research on thin-walled structural beams, and is involved in NCSA's Computational Extension (CompEx) Program to take advanced computing methods to small- and medium-sized businesses throughout the State of Illinois.

What is finite-element analysis?

Finite-element analysis is a CPU-intensive modeling technique for solving a variety of engineering problems that range from structural analysis to fluid flow. Finite-element methods enable engineers to construct models that behave realistically. Used to design items ranging from folding chairs to cars and space shuttles, FE programs generate the familiar mesh-like computer models often seen in TV commercials.

There is reason for the wire mesh appearance of FE models. Finite-element programs work by sectioning a large object into numerous small elements with simple geometries to make a complex problem easier to solve. Physical properties are also assigned to the model via the elements. Just as a magazine color photo is comprised of numerous dots—each with a specific color—a finite-element model is comprised of numerous elements with specific values. In FE analysis, the elements are linked—what happens to one element will affect the elements near it, the ones near them, and so on.

Improved computers divide the model into more elements to increase realism. In fact, elements have become so numerous (up to 250,000 in some cases) that they are practically invisible in many models. Changing physical properties (such as stress) are shown in colors that seem to flow across the model. High-speed computers have revolutionized the use of FE because they have increased the accuracy of computer models, enabled engineers to model more complex problems, and increased the speed and manner in which testing occurs by reducing the need to build prototypes. Costly mistakes are also avoided.

Some of Ahmad's work with FE codes centers around his own research on thin-walled structural beams. He studies the coupling between torsion and flexure (bending and twisting) properties in various designs. "The most common structural beam is the I-beam," says Ahmad, "but many are far more complicated than that."

***Fouad Ahmad** continued on page 8*

Fouad Ahmad continued from page 7

Ahmad's discovery of NCSA

Ahmad's initial acquaintance with NCSA came through an ***access*** article that he saw in late 1988 while teaching at the University of Wisconsin at Milwaukee. A student showed him a story about NCSA's free 1-hour test drive on the CRAY X-MP/48 [see ***access***, September–October 1988]. Since NCSA had just switched to a UNIX-based operating system, which Ahmad already knew, he decided to take advantage of the offer. He was so enthused he immediately introduced his classes to supercomputing. In the summer of 1989, he attended the Supercomputer Education Workshop conducted and organized by Nora Sabelli to learn better ways to present supercomputing to his students [see ***access***, September–October 1989].

Fouad Ahmad. (Photo by John Melchi, Information and Publications Group.)

"It provided extensive training that I took back to my students in Wisconsin," says Ahmad. To compare speed and results, Ahmad had his students work one problem on three computers—an IBM PC/AT, a MicroVAX II, and the CRAY X-MP/48. Since many of his graduate students had jobs in the field, he encouraged them to bring in problems from work. "The enthusiasm of my students increased dramatically when they began to work on real problems instead of exercises."

Many of Ahmad's students worked for companies too small to own supercomputers, and some of his colleagues questioned the wisdom of exposing students to a tool they might never use. They feared that students would become discouraged. Ahmad disagrees. "Even if a student's workplace does not have a supercomputer, the student still learns by using it. Besides, the advancement of technology is such that eventually he may have the power of today's supercomputers on his desktop. When that time comes, he'll be ready."

Computers and people

"Networked computers offer us a unique ability to communicate with each other," Ahmad continues. "With them we can work on projects jointly, send and receive messages, or talk halfway around the world. I believe we should use the technology to build relationships with colleagues and make work an enjoyable place to be. If society is impersonal, it's our fault—not the computer's."

Ahmad's code evaluation work ties in nicely with the Cray Applications course he teaches to NCSA users. "I'm one of the heaviest users of finite-element codes here," says Ahmad, "and that's a tremendous advantage when you're showing others how to run them." Ahmad conducts FE training sessions during each of NCSA's New User Applications Training workshops. Lyle Rigdon, manager of NCSA's Training Program who coordinates the workshop, says Ahmad's "understanding of the technology is extremely strong. Best of all, he truly cares about his audience. He finds out ahead of time who will be in the class and what specific problems they are working on, then he tailors his course to their needs. We are grateful to Fouad for his support and commitment to our user group training program."

Another of Ahmad's roles is with NCSA's CompEx Program, an initiative funded in the recent technology challenge grant competition, that is designed to help small- and medium-sized businesses with advanced computing. NCSA is working with the city of Effingham as a case study; the goal is to assist small- and medium-sized businesses through supercomputing usage. As part of the program, Ahmad is helping Effingham consortium member World Color Press optimize a printing press using finite-element analysis.

Changes and research

Although his first name is Mohammed, Ahmad chooses to use his middle name, Fouad. "In Egypt everybody is named Mohammed," says Ahmad. "Yell Mohammed in a crowded room, and everybody turns around. So I go by Fouad." Born in Cairo, Ahmad attended Cairo University and graduated with a bachelors degree in civil engineering in 1972. In 1980 Ahmad earned a master's degree from the University of Newfoundland and in 1984, a Ph.D. in theoretical and applied mechanics from the University of New Hampshire. Ahmad accepted a position at the University of Wisconsin at Milwaukee in 1986 where he taught and conducted research prior to joining NCSA.

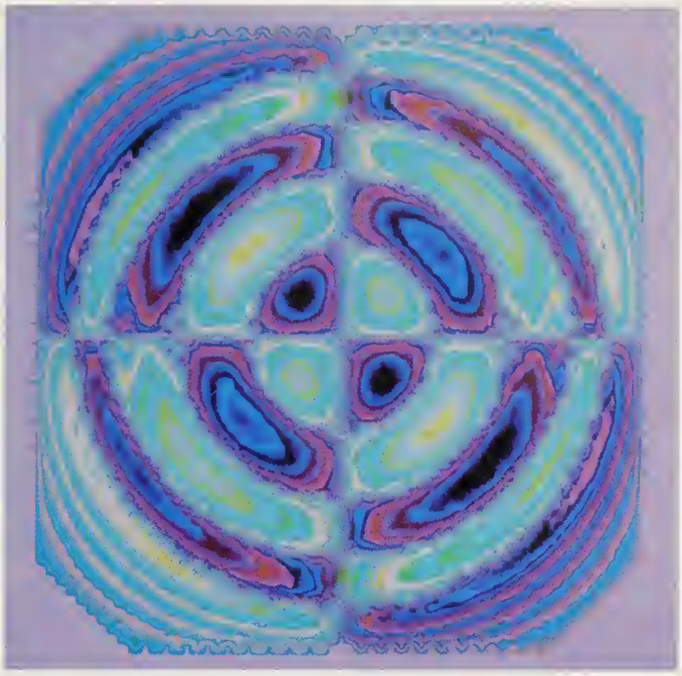
"It's a wonderful thing to have so many people from different disciplines in the same building," says Ahmad, who is especially looking forward to continuing work in the Beckman Institute. "This is truly unique. There is tremendous potential for cooperation between the sciences here." ▲

Scientific visualization: like playing piano

by John Melchi, Public Information Intern

A pioneer program in computer graphics at Parkland Community College is being offered to meet the demand for specialized technicians to visualize data generated on high-performance computers. Students are trained to create images on a computer graphics workstation by turning numerical data into graphic simulations. The 1-year vocational program is the nation's first [see ***access***, May–June 1989], and it is graduating a new generation of technicians schooled in computer graphics who are ready for the competitiveness of jobs in science and industry.

Students are experiencing teamwork on visualization projects by assisting NCSA industrial partners like Motorola, Inc. They evidence a natural propensity for art and science and communicate an enthusiasm for scientific visualization.



Electromagnetic field generated by a dipole in free space visualized by Motorola interns David Bennett, Ron Carbonari, Don Colby, and Sharon Yeakel. (Courtesy Motorola, Inc.)

Retooling for a career change

By age 5, Don Colby was already learning to play the piano. In elementary school he played the string bass. As an adult he taught music history and string bass at the University of Texas–El Paso. Colby's love for music and art eventually conceded to the demands of raising a family of five, so he returned to Illinois where he later began working on industrial computers.

In 1988 at age 42, Colby left the work force as a digital computer mechanic at Chanute Air Force Base in Rantoul to attend college full-time. Colby soon discovered the computer graphics program at Parkland and decided to pursue two lifelong pleasures: art and science.

Colby is one of 13 students expected to graduate from the "Advanced Certification Program for Visualization Computer Graphics Specialist," says Program Director Dick Bennett. Bennett recently replaced Sunny Christensen, who conceived and developed the original proposal and set up the program, bringing together the institutions and personnel involved.

Like other students, Colby has completed demanding courses in computer graphics taught at Parkland and at the Beckman Institute's Renaissance Experimental Laboratory (REL) by Ray Idaszak and Mike Krogh, NCSA graphics specialists.

"I gain as much pleasure from going to the Beckman Institute and sitting down at a Silicon Graphics Personal IRIS Workstation as I do when I go home and play my piano," Colby says ardently.

He is also collaborating with Bruce Litchfield, UIUC assistant professor of agricultural engineering, who is processing MRI data using the Cray supercomputers to study transport phenomena in foods during their processing. When the research is complete, Colby will visualize the data. He is now studying agricultural engineering and computer science at UIUC.

In addition to meeting prerequisites and completing 12 courses, students are involved in comprehensive internship projects in collaboration with NCSA scientists and other researchers. Colby, David Bennett, Ron Carbonari, and Sharon Yeakel worked as an internship team for NCSA's industrial partner Motorola. They created a set of images used in a company video presentation.

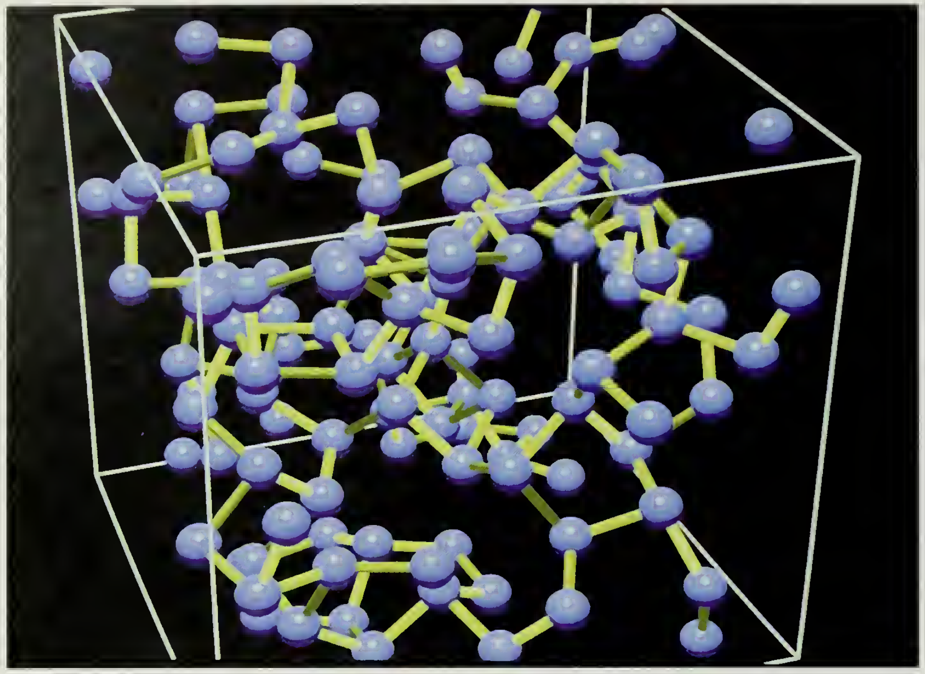
Imaging for Motorola

According to Margaret Nadworny, Motorola's engineering applications liaison at NCSA, the students used Internet and the resources at REL to discover existing tools in the public domain, putting together software used for the Motorola project. The students created time-elapsed images of an electrical field generated by a dipole disturbance from an electromagnetic program. The resulting visualization demonstrated to management and engineers how the software program treats well-understood problems. A basic problem was chosen so the visualization would be clearer to the viewers.

"The visualization increases the power of the computer simulation," Nadworny says. "The purpose was to show higher management that this program and visualization can be used to solve problems of interest to Motorola.

"The students were very enthusiastic. We were impressed with that. We found that their visualization knowledge was very good," she adds. "They were willing to do anything, at any time, under any circumstance. That was very nice. It was refreshing to me.

Scientific visualization *continued on page 10*



Molecular dynamics image of a 124-atom phosphorous configuration visualized by Dave Bock.

Three-dimensional image of data representing sensory responses to four different breads by Don Colby.

Scientific visualization *continued from page 9*

"One expectation of our partnership with NCSA is to transfer visualization expertise, techniques, and capabilities into our company. We want to be exposed to and participate in all the programs available to us at NCSA in order to accomplish that aim," Nadworny said. "Motorola is an industrial partner because we believe supercomputing, visualization, and good science and engineering all play a role in our future as a company."

Starting over with enthusiasm

David Bennett, 43, former business systems director at an extended care facility, also left the workforce to pursue a career in scientific visualization. "I have not regretted it since," he says. "Visualization is the most exciting field out there. I feel like I'm 18 and starting all over again."

In August Bennett accepted a position with the North Carolina Supercomputing Center at the Research Triangle Park as a visualization technician. He will be developing software, providing technical support for researchers and industrial partners, as well as doing visualization. One of Bennett's visualization projects in North Carolina is to assist the Environmental Protection Agency in their study of acid rain and its effect on the environment.

"The enthusiasm of NCSA, the instructors and their dedication and love of doing visualization really helped us. They gave us a lot of support," he says. "Sunny Christensen was an our principal motivator and helped provide stability in a new environment."

Two other students in the program, Jan Moorman and Jean Ascoli, are continuing their education at UIUC. Moorman will pursue a master's degree in computer science and Ascoli a master's degree in architecture. The remainder of the students are finishing their internships and are being assisted by Dick Bennett and Sunny Christensen in finding positions.

This past summer the class expanded their horizons by attending SIGGRAPH '90 to establish potential employment contacts and to learn more about computer graphics through participation in conference activities. "We came back enthused," says Bennett. To continue the momentum, Bennett and several students operated a promotional display of student visualizations on a graphic workstation at the Illinois State Fair the week after SIGGRAPH. The display was done in collaboration with IBM.

Focusing in on visualization

While reading an issue of *Byte* magazine, Dave Bock first encountered scientific visualization and NCSA. Even though the 26-year-old had graduated from Southern Illinois University–Carbondale in 1987 with a bachelor's in electrical engineering and was already working in that field, he decided to look for a position in computer graphics.

"Just about the time I was ready to give up as I looked for a job in computer graphics," says Bock, "I heard about the Parkland program from a friend. This program is so specific; it is so focused that you know what you will be doing in the end. Because of that, it is exciting. I enjoyed it."

Today Bock is involved in interactive visualization research at Aviation Research Laboratory, UIUC. Bock is determining if the visualizations are answering the questions they were expected to. "I always thought that work was something that had to be monotonous every day," he says. "If that's work, this isn't work." ▲

New user training evolves at NCSA

by Lyle Rigdon, Manager, Training Program, and Jarrett Cohen, Public Information Specialist

Through surveying our academic and industrial users, NCSA has redesigned the Training Program. We now offer three types of modularized training programs to the user community on a monthly rotational basis as follows: Cray applications, Cray code development, and Connection Machine code development. Modules on scientific visualization are a vital part of each session.

Training in scientific visualization

A core element of the training provided by NCSA is scientific data visualization. As the size of computable problems has grown, so has the difficulty in dealing with the amount of data produced. For example, recently a researcher was interested in visualizing forest fire data from Yellowstone National Park derived over 300 years [see ***access***, May–June 1990]. Through the use of data visualization techniques, the researcher was able to see the effect that past fires had on plant life within Yellowstone, to make "what if" statements with the data, and then to view the visualized results. This is one example of many types of simulations and scientific modeling that are currently possible. The Cray visualization training module covers the following topics: Introduction to Data Visualization, Cray Graphics, HyperCard Animation, Introduction to Raster Graphics, NCSA Scientific Visualization Software Suite for the Macintosh, Hierarchical Data Format (HDF), and Media Output.

Cray applications training

This 3-day session is geared toward researchers who are interested in running the applications packages resident on NCSA's Cray systems. An introduction to NCSA and UNICOS will be provided, followed by parallel sessions on a variety of applications in the fields of chemistry, finite elements, and computational fluid dynamics. Within these areas, attendees will become aware of which application software packages are available and their relative performance characteristics. A full day of scientific data visualization is also included. Hands-on laboratories are provided. As a prerequisite, familiarity with UNIX and Macintosh systems is suggested.

Cray code development training

Beginning in a fashion similar to the Cray applications course, this 5-day session also offers an introduction to NCSA and UNICOS. Cray code development training differs from the applications course in that the focus is on empowering participants with the tools and knowledge that will increase the performance of participants' codes on the Crays. Advanced topics include Vectorization, Numerical Libraries, Debugging Codes, Optimization, and Timing Tools. This course requires a strong familiarity with Fortran and a working knowledge of the UNIX operating system and Macintosh computers. Hands-on laboratories are provided.

Connection Machine code development

This 5-day session on the Connection Machine Model 2 (CM-2) covers the emerging technology of massively parallel computing. Topics to be covered include Introduction to Data Parallelism, Scientific Computing on the Connection Machine, Connection Machine Architecture, Data Structures, Operations and Low-level Algorithms, Connection Machine I/O System, Efficient Algorithms for Number Computations, Introduction to Connection Machine Fortran, Introduction to C/Paris, I/O Programming, DataVault, and Graphics Capabilities. Hands-on laboratories are provided. A mastery of UNIX and Fortran is expected of participants.

For further information, contact Lyle Rigdon [see **NCSA contacts**, page 19]. ▲

Tentative training dates: 1990–91*

1990	
December 3–5	Cray Applications Training**
1991	
January 14–16	Cray Applications Training**
February 18–22	Cray Code Development Training
March 18–22	Connection Machine (CM-2) Training
April 15–17	Cray Applications Training**
May 13–17	Cray Code Development Training
June 17–19	Cray Applications Training**
July 15–19, 22–26	Connection Machine (CM-2) Institute
August 19–23	Cray Code Development Training
September 16–18	Cray Applications Training**

You must register to attend NCSA Training. Class size is limited.

To register: Academic users contact Karen Gobble at (217) 244-4198. Industrial partner users contact your representative at NCSA.

***NOTE:** These dates are subject to change.

**Applications will be in the fields of chemistry, finite element, and computational fluid dynamics.

Computational Science in Education Workshop

by James Toepper, Staff Assistant

Preparation for the Computational Science in Education Workshop is underway. The workshop is funded by NSF and will be held October 28–30 to discuss ways that high-performance computing centers can promote computational science and engineering (CS&E) in the education of precollege, college, and university students [see ***access***, July–August 1990]. Target audiences for the workshop recommendations include educational institutions, high-performance computing centers, and funding agencies.

As a first step in gathering a group of panelists for the October workshop, a steering committee met at the Beckman Institute August 16. Names of the steering committee are in the right column. Melvyn Ciment, deputy director, Division of Advanced Scientific Computing at NSF, joined the group. Three participating strategic vendors asked to express industry's education viewpoint at the October workshop were represented by Michael Condry, AT&T; Bernie Rudin, IBM; and Tim Whitley, CRI.

The steering committee selected a panel of 30 participants. The panel will maintain a balance among several areas: scientific disciplines; agency affiliation; precollege, college, and graduate education; and minorities underrepresented in science and engineering. Two staff associates have been chosen to work with Nora Sabelli on background studies for the workshop—Ann Solem, Los Alamos National Laboratory, and Robert Panoff, Clemson University.

Other action included developing a longer list of contacts for the data collection process and setting guidelines on background studies to be undertaken by the panel staff associates in October.

Three working groups composed of the panel staff, NSF-sponsored supercomputer centers, and strategic vendor representatives will conduct a series of data gathering background studies for the October workshop. These studies will not be full-fledged reports—rather, broad surveys to provide data on the education community successes and needs for CS&E education on which to base workshop discussions and recommendations.

If you are interested in the work of the panel by providing examples of successful programs that could be emulated, pitfalls to avoid, or in collaborating on the background studies, contact Nora Sabelli, senior research scientist at NCSA [see **NCSA contacts**, page 19] or any other steering committee member. ▲

Steering committee

Larry Smarr, director, NCSA, *principal investigator*

Nora Sabelli, senior research scientist, NCSA, *panel coordinator and co-principal investigator*

Maha Ashour-Abdallah, professor of physics, UCLA, and member, Program Advisory Committee of Division of Advanced Scientific Computing

Helen Doerr, associate director, Cornell National Supercomputer Facility, *panel working group*

Michael Haney, president, National Consortium for Specialized Secondary Schools of Mathematics, Science, and Technology

Karen Johnston, professor of physics, North Carolina State University

Larry Lee, director, North Carolina Supercomputing Center

Richard Mandelbaum, provost, University of Rochester

Rozeanne Steckler, staff scientist, San Diego Supercomputer Center, *panel working group*

Robert Stock, manager of User Services, Pittsburgh Supercomputing Center, *panel working group*

Software

NCSA software updates

by Jill Peacock, Editorial Assistant, Software Tools Group

NCSA's Software Tools Group (STG) recently released two new software packages for the Silicon Graphics Workstation as well as an application which converts non-HDF files into HDF files. HDF (Hierarchical Data Format) is a multiobject file structure.

In addition, STG has released updated versions of various scientific software packages that are more versatile in their enhanced versions.

NCSA PolyView 1.0 for the Silicon Graphics Personal IRIS Workstation is an interactive visualization tool for HDF Vset data. HDF Vset allows you to work with a wide range of data, including mesh data, vertex and polygonal data, Lagrangian meshes, irregularly gridded data, finite-element data, and 3D graphical data. NCSA PolyView displays an HDF Vset of polygons, or points, as a 2D or 3D interactive image with optional annotation, which may be written to an HDF raster format file. The program allows you to (1) interactively manipulate and display objects; (2) render images as points, lines, or polygons; (3) choose constant or gouraud shaded polygons; (4) load and manipulate the color map; (5) animate time series data; (6) view a flyby of the data using a script file; and (7) pick subregions and get original data values. (See the PolyView article on page 14.)

NCSA HDF 3.1 Hierarchical Data Format (HDF) is a multiobject file format for the transfer of graphical and floating-point data between machines. The design of this format enables self-definition of data content, and easy extensibility for future enhancements to or compatibility with other standard formats on the Hierarchical Data Format developed at NCSA. Changes in this version include the following:

At SIGGRAPH '90. Joseph Hardin (left), manager of NCSA's Software Tools Group, briefs editors Nicolas Mokhoff (center) and Richard Wallace (right) of *Electrical Engineering Times.* (Photo by David Curtis, Information and Publications Group.)

(1) added functions, including `DFR8readref`, `DF24readref`, `DFSDreadref`, and `DFPreadref`, which permit random access by reference number; (2) new functions `DF24restart` and `DF24setil`; (3) increased speed in `DFSDgetdata`, `DFSDputdata`, `DFSDadddata`, `DFSDgetslice`, and `DFSDputslice` functions, especially for UNICOS systems; (4) additional annotation functions: `DFANaddfid`, `DFABaddfds`, `DFANgetfidlen`, `DFANgetfid`, `DFANgetdslen`, `DFANgetfds`, `DFANaddfann`, `DFANgetfannlen`, `DFANgetfann`, and `DFANlastref`; (5) a revision of `DFANlablist` so that it returns all reference numbers for a given tag, regardless of whether or not there is a label; (6) elimination of a bug with `DFSDgetdata`; (7) additional macros to make passing character arrays from Fortran to C easier; (8) bug repairs; and (9) recoding of some areas for easier readability.

NCSA Import2HDF 1.0 for the Macintosh is a tool developed to enable users to convert non-HDF files to HDF files. Once the files are converted, users can utilize NCSA-developed software or other software that works with HDF format files. NCSA Import2HDF also allows users to change labels associated with elements of HDF files. For instance, you can assign or alter labels for each Raster Image Set (RIS) or Scientific DataSet (SDS) that an HDF file contains. NCSA Import2HDF also displays RISs and SDSs. Other features of the program allow you to (1) convert FITS, TIFF, GIF, raw raster image, and ASCII files to HDF format; (2) display the contents of HDF files; (3) display RISs in the form of color raster images; and (4) display SDSs in spreadsheet fashion.

NCSA Isosurface Visualizer 1.0 for the Silicon Graphics 4D Series Workstation is a noninteractive batch utility that enables users to easily create and view animations of isosurfaces derived from 3D data. Input data consists of a single 3D scalar array of floating-point values. Indices of this array form the x, y, z coordinates; the variable at each node determines where the isosurface passes through the data. Program features allow you to (1) control orientation of geometry, including independent x, y, z translation, rotation, and scaling; (2) control light source parameters, including arbitrary x, y, z location of light source and RGB color of light source; (3) specify material properties, including ambient, diffuse, and specular coefficients and specular high-light size, which allows control over how the light source interacts with the viewed object; (4) save hardware-rendered images to disk for 3D rendered animation sequences (including full hidden surface removal); and (5) save polygonal isosurfaces in either NCSA HDF Vset format for use and viewing with PolyView [see ***access***, May–June 1990] or in ASCII format.

NCSA DataScope 2.0 for the Macintosh now features new distributed capabilities across TCP/IP network connections; thus, NCSA DataScope is no longer limited to the processing power of the Macintosh alone. In addition, notebook functions can now automatically be executed on a remote machine. Although you do have to wait for the data to be sent there and back, this inconvenience is negligible when compared to the increased computational speed of the supercomputer. Specifically, the new network functions allow you to (1) send datasets from your mainframe to DataScope on demand from a mainframe application that you have written and (2) use a remote machine to access notebook functions that are too time-consuming to calculate or that you cannot compile on your Macintosh.

NCSA PalEdit 1.2 for the Macintosh is an interactive palette creation tool that helps you produce color palettes tailored to your needs. NCSA PalEdit version 1.2 contains a new tool, the selection tool, which allows you to make range selections in the component plot. This tool also allows adjustment of the selected range. Moreover, several tools and commands that modify a range of the palette now distinguish between modifying the whole color or just the actual component of colors. In addition, NCSA PalEdit version 1.2 offers the option of saving new or modified palettes in the following file formats: raw palette, HDF, Klutz DA, Canvas, and PixelPaint. Finally, a straighten option has been added to the Edit menu, which performs a linear interpolation between the end values of the active color component in the selected range to create the "smoothest" palette possible.

NCSA software can be obtained by downloading it by anonymous file transfer protocol (FTP) if you are connected to Internet (or NSFNET, MILNET, etc.). You can also receive the software via U.S. mail or the archive server.

FTP: (1) Log on to Internet host. (2) Enter **`ftp.ncsa.uiuc.edu`** or **`ftp 128.174.20.50`**. (3) Login as **`anonymous`**. (4) Enter your local login for a password. (5) Change directories if needed. (6) Enter **`get README.FIRST`** to transfer the instructions (ASCII) to your local host. (7) Enter **`quit`** to exit FTP and return to local host. (8) Review the **`README.FIRST`** file for instructions on downloading files.

U.S. mail: To order software developed at NCSA, see the September 1990 *Technical Resources Catalog* for instructions. Order forms are included in the publication. Contact the NCSA receptionist at (217) 244-0072 for additional copies. If you are not connected to Internet, telephone "Orders for user publications and NCSA software" [see **NCSA contacts**, page 19].

Software updates *continued on page 14*

PolyView, a next-generation visualization tool

by Scott Piette, Industrial Consultant, Industrial Program

Have you ever had the frustration of trying to display data that was calculated by using an irregular grid? Writing programs that convert data to fit into a regular grid so that it can be converted into images and displayed with an NCSA software visualization tool is time consuming. This process could cause a lot of frustration and reduce the spatial accuracy of your data.

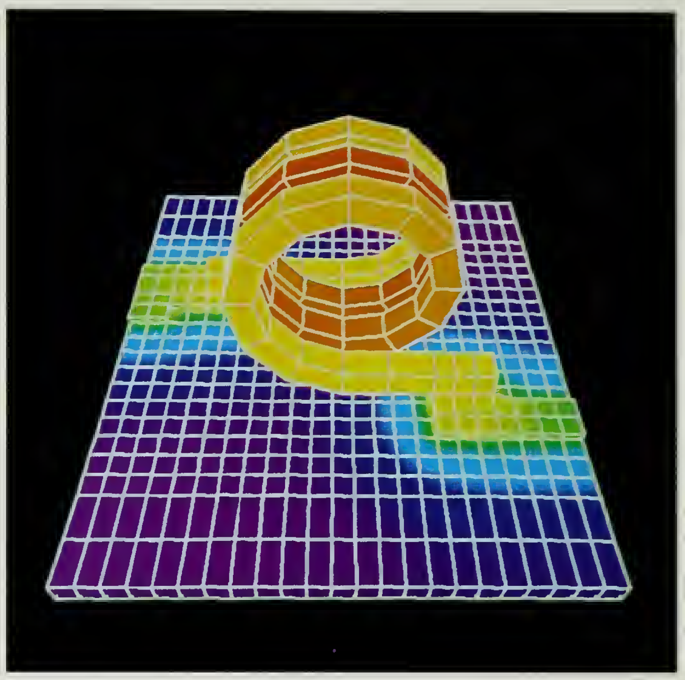
With the recent release of NCSA PolyView Version 1.0 and the NCSA Vset libraries, you will no longer have to waste time iterating through the image-generation process only to find that your images do not have the spatial resolution or accuracy you desired.

Developed by the Software Tools Group, NCSA PolyView was recently released for Silicon Graphics, Inc. Personal IRIS workstations. PolyView enables users to create two- and three-dimensional representations of datasets and interact with their images. (For further details, see "NCSA software updates" on page 12.)

NCSA PolyView derives its name from the term "Polygon Viewer." Its ability to represent polygons makes PolyView unique. Most visualization tools work only with regularly gridded information, which means they can only plot points that fall on regular coordinates, such as (1,1), (1,2), (2,2), etc. But PolyView can work with irregularly gridded information, such as in finite-element methods, and plot points or polygons at any coordinate, (1.6, 2.3) for instance.

Unlike previous NCSA-produced tools, PolyView uses the new HDF Vset format. With the Vset format, users are able to store several sets of floating-point values for each point—the x, y, and z locations for each point. A connectivity list describes how the points are connected to form polygons. By saving all this original information, users never have to go back to the original simulation.

One of the earliest uses for NCSA PolyView was to study the thermal properties of a heated coil. A coil was modeled with 9,189 elements outlined in white. PolyView was used to study the heat patterns as the coil heated from room temperature to 90°C. By using PolyView, the palette was interactively changed to identify the problem areas. The image above shows the final state of the coil. Red areas identify the areas of high temperature, while blue areas represent the cooler regions. ▲



Slice of a coil heating up displayed with NCSA PolyView Version 1.0. Using a finite-element method, 9,189 elements (outlined in white) were modeled. (Courtesy Scott Piette.)

Software updates *continued from page 13*

Archive server: You may obtain NCSA software via an archive server by (1) sending electronic mail to **`archive-server@ncsa.uiuc.edu`**. (2) Include in the subject or message line, the word **`help`**. (3) Send another message containing a line with the word **`index`**.

For example, if you use the UNIX mailing system, your login session should resemble the following sample, where user entries are indicated in boldface type.

```
yoyodyne_51% mail archive-server@ncsa.uiuc.edu
Subject: help
.
EOT
Null message body; hope that's ok
yoyodyne_52% mail archive-server@ncsa.uiuc.edu
Subject: index
.
EOT
Null message body; hope that's ok
```

Note: This is a controlled access server that will electronically mail the distribution to you one segment at a time. It will gateway to BITNET and overseas. ▲

Industrial Program looks to the future

by Jarrett Cohen, Public Information Specialist

NCSA's Industrial Program, now entering its fifth year, must evolve to meet its partners' changing needs, says Corporate Officer John Stevenson. With many of its partners approaching the end of their initial 3-year agreements and one partner (Eastman Kodak Company) having already renewed twice, the Industrial Program recently changed its organizational and pricing policies.

When corporations first join NCSA's Industrial Program, they are usually inexperienced in the use of supercomputing systems and technology. Therefore, rather than just supplying supercomputer cycles, NCSA provides a comprehensive program that immerses corporate users in high-performance computing. Aside from supercomputing time, major components of this program include scientific visualization, training, networking, applications support, consulting, hardware, and software.

As would be expected, partners' use of NCSA supercomputers starts off rather slowly—particularly in the first year—and then ramps up after they have learned to use the systems and have chosen specific applications. Along with increased supercomputer usage, the need for more specialization arises.

Advanced Partnerships available

In addition to NCSA's Associate and Full Partnerships, there is now an Advanced Partnership. This latter partnership is for those corporations staying on beyond the first 3 years or those corporations that have their own supercomputer and significant experience with computational science.

Advanced Partners have more flexibility in that they choose the components of computational science for which they want support. For example, Company X may want supercomputing time, visualization, and applications support, while Company Y may request supercomputing time, applications support, and software development.

New pricing policies

NCSA also recently changed its pricing practices for supercomputing time. Previously, there was a flat rate regardless of the amount of usage. A cost and usage study showed that this procedure placed too much burden on the partners in their years of advanced usage—a time when they are often using several thousand hours.

The new pricing scheme takes a three-tiered approach with successively lower prices at each level. Prices are charged in terms of billing units per year, which are figured by a different algorithm for each machine.

"This new system better matches partners' needs and makes us very price competitive," says Stevenson; however, the levels of partnership have not been changed, Stevenson stresses. For instance, a corporation must still commit to a minimum 3-year, $3 million agreement to become a Full Partner.

For further details, contact John Stevenson, associate director of the Industrial Program [see ***NCSA contacts***, page 19]. ▲

Eastman Kodak extends contract with NCSA

by John Stevenson, Associate Director, Industrial Program

NCSA is pleased to announce that the Eastman Kodak Company signed an agreement that establishes them as the center's first Advanced Partner in the Industrial Program. The agreement confirms their continued participation as a Full Partner for the rest of calendar year 1990 and initiates the Advanced Partner relationship for calendar year 1991.

Kodak originally joined the Industrial Program in August 1986, for 3 years, then extended their contract from August 1989 to December 1990. The extension we are announcing brings Kodak's involvement at NCSA to over 5 years.

For the remainder of 1990, Kodak will be concentrating at NCSA on increasing supercomputer usage on all of the center's systems; training new users; working with their new consultant, Jim Ferguson, to help them solve technical user problems; and increasing applications expertise in computational chemistry and computational fluid dynamics. ▲

Gigabit-per-second network R&D

by Charlie Catlett, Manager, Networking and Systems Development

NCSA has received preliminary funding from the Corporation for National Research Initiatives (CNRI) for a 3-year project to develop gigabit-per-second network applications and programming environments. With funding from NSF and the Defense Advanced Research Projects Agency (DARPA), CNRI is establishing five major network testbed projects. The CNRI program is part of a national initiative in research and development that is aimed in part toward the implementation of the National Research and Education Network (NREN). Proposed for installation in the mid-1990s, the NREN would be a multigigabit fiber optic national network connecting universities, national centers, and corporate and government research facilities.

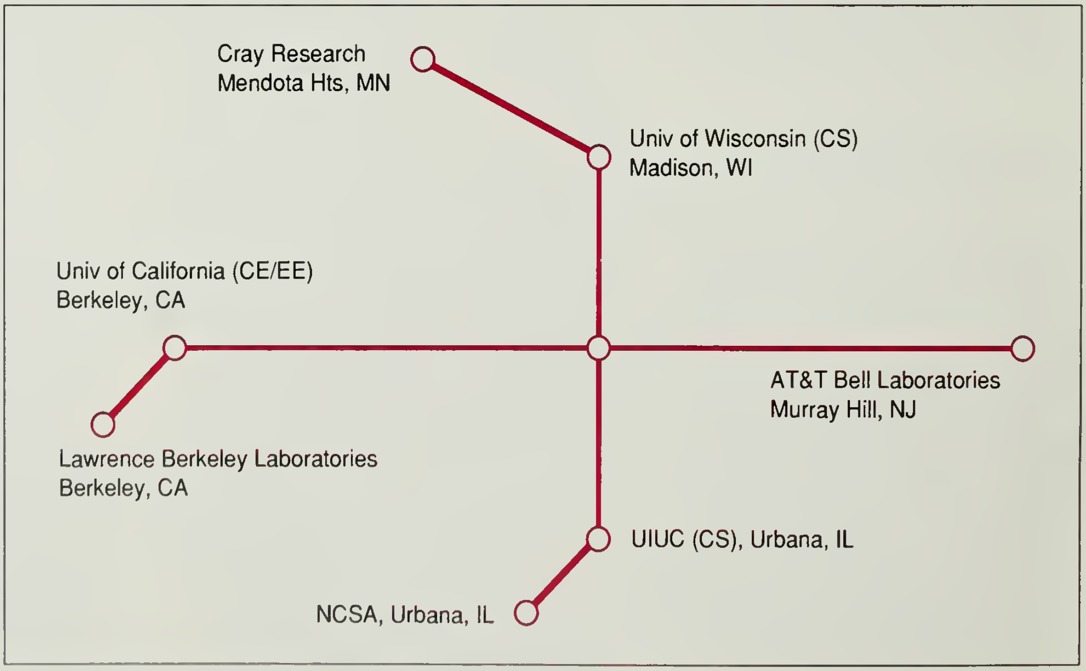
The NCSA research is part of the BLANCA testbed, a project that includes research and development in network architectures, protocols, and high-performance applications. The work will be carried out by NCSA, AT&T Bell Laboratories (Murray Hill, NJ); the UIUC Department of Computer Science; the University of Wisconsin at Madison Department of Computer Science and Space Sciences and Engineering Center (SSEC); the University of California at Berkeley Department of Electrical Engineering and Computer Science; and Lawrence Berkeley Laboratories.

BLANCA will use network facilities that are part of an AT&T-funded network research project called XUNET. The network, currently running at 1.5 megabits per second, will be upgraded to 45 megabits per second this year. By the end of 1991, the link between NCSA/UIUC and the University of Wisconsin at Madison will be upgraded to 622 megabits per second.

In addition to AT&T facilities, the XUNET network includes cooperation with Ameritech, Bell Atlantic, and Pacific Telesis. An extension of the XUNET network is planned to provide a link to Cray Research, Inc. in Mendota Heights, MN. The extension will be provided by Norlight. (See figure below.)

NCSA applications activities as part of BLANCA will include the development of a distributed programming environment that supports interactive visualization by several researchers concurrently. The Distributed Interactive Collaboration Environment (DICE) is a new visualization and general programming environment built on an NCSA-developed general message-passing system. DICE is specifically designed to support real-time collaboration by multiple, widely dispersed scientists through such capabilities as shared control and viewing of simulation output.

In addition, NCSA research scientists and technical staff will work with collaborators at other BLANCA sites to evaluate various network architectures and to develop network protocols necessary to support applications throughput of over 500 megabits per second. Several approaches will be explored, including the implementation of extensions to the Transmission Control Protocol (TCP) and the use of network virtual memory schemes. ▲



The BLANCA testbed uses network facilities that are part of the AT&T XUNET Network Research project.

CRAY Y-MP migration

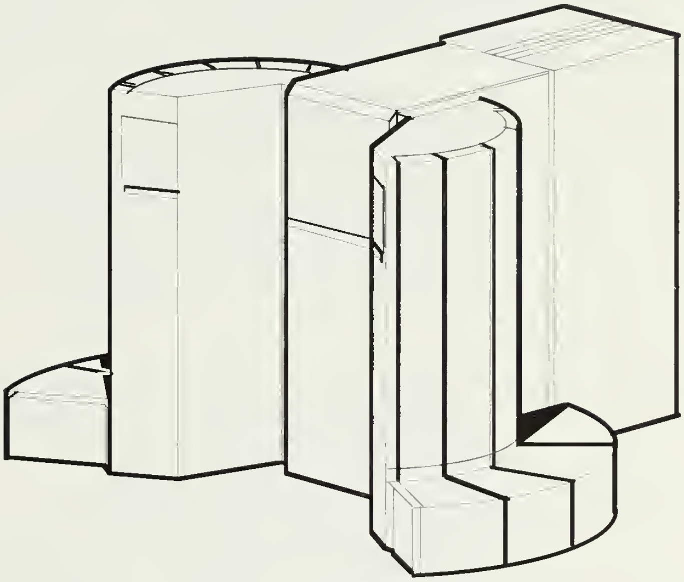
by William Dwyer, Graduate Assistant Writer

A new 4-processor CRAY Y-MP system with 64 megawords of memory is scheduled to arrive for installation in mid-October. Planning for the migration from the CRAY X-MP system to the CRAY Y-MP system is in progress. Users will receive a migration guide in the mail around mid-October.

The UNICOS operating system will continue to be used on the new system; CRAY X-MP programs can be used on the CRAY Y-MP system in X-mode without recompiling, although recompiling will improve performance in many cases.

Shakedown of the new system is scheduled during the 2 weeks following installation, after which the CRAY X-MP system will be removed. Watch online news and documentation for updates or contact the Consulting Office [see **NCSA contacts**, page 19]. (The CRAY-2 system will stay at NCSA and will not be affected in the transition.)

Users are encouraged to apply for allocations on the new machine. Proposals must be in by November 1 for consideration at the December Peer Review Board and the Small Allocation Committee meetings. Contact Patricia Wenzel, manager of Client Administration, for procedures [see **NCSA contacts,** page 19]. ▲



The CRAY Y-MP supercomputing system.

Center cache

Several awards and appointments were recently announced at NCSA. They are as follows:

David Ceperley, NCSA research scientist and UIUC associate professor of physics, recently won a Xerox Faculty Award for his research in quantum physics. This award recognizes Ceperley's contributions to simulation methods for many-body systems.

Donna Cox is now associate director of the Numerical Laboratory Programs. (Formerly she was associate director of Education.) Cox is also a UIUC associate professor of art and design.

Zhi-Pei Liang, postdoctoral fellow in NCSA and the Biomedical Magnetic Resonance Laboratory of the University of Illinois College of Medicine at Urbana–Champaign, together with coauthors E. M. Haacke and S. H. Izen, has been awarded the Sylvia Sorkin Greenfield Award for the best paper published in 1989 in *Medical Physics.* Entitled "Constrained Reconstruction: A Superresolution Optimal Signal-to-Noise Alternative to the Fourier Transform in Magnetic Resonance Imaging," the paper was based on Liang's Ph.D. dissertation.

Melanie Loots is now Assistant Director for Engineering Applications. Until recently, she was staff associate for the Applications Group.

Marcia Miller has joined the Applications Group as Assistant Director for Applications Software and will work with NCSA's managers to develop a comprehensive process for the acquisition, installation, and support of software. Miller was formerly assistant deputy director for Science, Technology, and Education. ▲

New and updated online information

by Will Ridenour, Online Documentation Editor

The following help files, man pages, and documents have been added or updated as of September 4, 1990.

UNICOS help files

Name	**Description**
contacts	Contact person for information about specific areas
software	The latest list of software installed and planned on NCSA machines
training	Information about NCSA user training

ULTRIX help files

Name	**Description**
contacts	Contact person for information about specific areas
conversion	Information about using ncsagate
software	The latest list of software installed and planned on NCSA machines
tapes	Information about reading and writing tapes at NCSA
training	Information about NCSA user training

To access a help topic on either Cray system or ncsagate, enter **`help`** ***`topic`***, where *topic* is the name of the topic you wish to view.

UNICOS man page

Name	**Description**
bcs	General-purpose math library
bcsext	Out-of-core and sparse solver library
top	Displays process and Network Queueing System (NQS) information

To access a UNICOS man page, enter **`man`** ***`manpage`***, where *manpage* is the name of the man page you wish to view.

UNICOS documents

Name	**Description**
scc.2.0.rm	Cray Standard C Programmer's Reference Manual
cft77.vol1	CF77 Compiling System, Volume 1: Fortran Reference Manual
cft77.vol4	CF77 Compiling System, Volume 4: Parallel Processing Guide

To access one of these documents, change directories to /usr/local/doc and enter **`more`** ***`docname`***, where *docname* is the name of the document you wish to view.

SIGGRAPH '90 *continued from page 6*

and hardware; disciplinary support, by sponsoring workshops; and by supporting supercomputer centers at "both ends and the middle." The NSF centers are "the leaders in scientific visualization across the country," Hirsh said.

The National Institutes of Health's (NIH) Advanced Scientific Computing Laboratory is the home of the first supercomputer dedicated to biomedical research. Jacob Maizel, Jr., director of that laboratory at the National Cancer Institute at NIH, said that one-half of the time on the soon-to-be-upgraded CRAY X-MP/24 system is allocated to outside researchers. NIH also supports medical imaging. ▲

Plasma physicist *continued from page 3*

Simultaneous with each movement through the lattice, there are two graphs shown. One represents position; the other shows velocity. In his summary, Ruzic explains that the manufacture of semiconductor chips is dependent on an understanding of plasma–surface interaction.

In November, Ruzic will visit several research laboratories in Japan and use the video to demonstrate his research. At scientific conferences, he plans on showing a shorter version. Henry Chiu, UIUC graduate assistant in nuclear engineering, worked with Ruzic on the research.

Learning the science

"Anytime we do a project, we have to educate ourselves about what we're doing—the science behind it," explains Mehrotra. While working with Ruzic, Mehrotra says he and Corson learned much about plasma–surface interaction as they determined how to graphically represent the scientific data.

Corson says her greatest challenge was "to compose the animation in a manner that would most strongly convey the information to both the researcher and the general audience. This involved experimentation with shadows, lighting, and camera motion."

Cordelia Baron, Bob Patterson, and Jay Rosenstein of NCSA's Media Services group collaborated with Corson and Mehrotra in postproduction of the 9-minute video. Rosenstein was in charge of audio, and Patterson was in charge of video editing. ▲

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Anonymous FTP IP address
ftp.ncsa.uiuc.edu (128.174.20.50)

CM Sun front-end address
cmsun.ncsa.uiuc.edu (128.174.220.4)

CM VAX front-end
cmvax.ncsa.uiuc.edu (128.174.220.5)

Cray operations
(217) 244-0710

CRAY X-MP IP address
ux.ncsa.uiuc.edu (128.174.10.46)

CRAY-2 IP address
u2.ncsa.uiuc.edu (128.174.10.44)

Dialup access—2400 baud or less
(217) 244-0662

Dialup access—9600 baud
(217) 244-6733

NSF Network Service Center
nnsc@nnsc.nsf.net

NSFNET problems
(617) 873-3400

SRI-Network Information Center
(415) 859-3695
nic.ddn.mil

VAX/ULTRIX gateway addresses
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data link contents

Hot tips and topics

Using CFS to save and retrieve files
by Chris Walquist, Student Consultant

More on ncsagate
by Chip Mayse, Student Consultant

Internetworking and high-level applications
by Chris Walquist, Student Consultant

CF77 version 4.0 now available
by Kurt Hirchert, Systems Consultant

New release from NCSA—HDF 3.1
by Mike Folk, Senior Programmer, and Chin-Chau, Graduate Research Assis

KAP/Cray—a performance enhancement tool
by John Larson, Senior Computer Scientist, Center for Supercomputing Rese and Development, and Sanjiv Shah, Senior Developer; Kuck and Associates

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